A compact skeletal mechanism for *n*-dodecane with optimized semi-global low-temperature chemistry for diesel engine simulations

Tong Yao^{1, 2, 3*}, Yuanjiang Pei⁴, Bei-Jing Zhong^{2*}, Sibendu Som⁴, Tianfeng Lu³, Kai Hong Luo^{1,5}

Abstract: A skeletal mechanism with 54 species and 269 reactions was developed to predict pyrolysis and oxidation of *n*-dodecane as a diesel fuel surrogate involving both high-temperature (high-T) and low-temperature (low-T) conditions. The skeletal mechanism was developed from a semi-detailed mechanism developed at the University of Southern California (USC). Species and reactions for high-T pyrolysis and oxidation of C₅-C₁₂ were reduced by using reaction flow analysis (RFA), isomer lumping, and then merged into a skeletal C₀-C₄ core to form a high-T sub-mechanism. Species and lumped semi-global reactions for low-T chemistry were then added to the high-T sub-mechanism and a 54-species skeletal mechanism is obtained. The rate parameters of the low-T reactions were tuned against a detailed mechanism by the Lawrence Livermore National Laboratory (LLNL), as well as the Spray A flame experimental data, to improve the prediction of ignition delay at low-T conditions, while the high-T chemistry remained unchanged. The skeletal

mechanism was validated for auto-ignition, perfectly stirred reactors (PSR), flow reactors and laminar premixed flames over a wide range of flame conditions. The skeletal mechanism was then employed to simulate three-dimensional turbulent spray flames at compression ignition engine conditions and validated against experimental data from the Engine Combustion Network (ECN).

Keywords: *n*-dodecane; surrogate; spray flames; ignition delay; skeletal mechanism

1. Introduction

Accurate prediction of diesel engine combustion requires realistic chemical kinetics. However, diesel fuels consist of a large number of components and involve an even larger number of intermediate species and reactions during the combustion process, and thus it is difficult to employ fully detailed mechanisms in practical engine simulations as the computational cost would be intractable. As a simplification, surrogate mixtures with one or a few components have been developed to mimic the physicochemical behaviors of the real diesel fuels [1]. Despite of the multi-component nature of diesel fuels, single-component surrogate can also be useful in predicting selected flame behaviors of diesel fuels at relatively lower computational cost compared with the multi-component surrogates. For instance, *n*-heptane has been widely adopted as a diesel surrogate [2-4]. The number of carbon atoms in practical diesel fuels can range from 10 to 25. Compared with *n*-heptane, *n*-dodecane features a molecular size close to that of average diesel components, and has been employed recently as a surrogate fuel to model diesel fuel combustion [5-15]. Moreover, *n*-dodecane features boiling characteristics in the mid-range of diesel fuels, hence is expected to better mimic the fuel-air mixing processes associated with spray evaporation than *n*-heptane. Detailed mechanisms for large hydrocarbons, e.g. *n*-dodecane, can consist of thousands of species and reactions when low temperature (low-T) chemistry is involved [16-20]. For instance, the detailed mechanism developed by Westbrook et al. [17] for *n*-alkanes from *n*-octane to *n*-hexadecane consists of 2775 species and 11,173 reactions. Such large mechanisms need to be reduced for computationally tractable three-dimensional (3-D) simulations.

Mechanism reduction has been extensively studied in the last few decades and a number of reduction methodologies have been developed [21]. Reduced mechanisms can be obtained by removing unimportant species and reactions from the detailed mechanisms and lumping of similar species and reactions, using such methods as reaction flow analysis (RFA) [22], sensitivity analysis [23-25], principal component analysis (PCA) [26], detailed reduction [27], directed relation graph (DRG) [28-31] and variants [32-34], path flux analysis (PFA) [35] and isomer-lumping [36,37]. However, reduced mechanisms for large hydrocarbon fuels with low-T chemistry obtained by such methods may still be large [5,38-42]. For example, a skeletal mechanism for *n*-dodecane developed by Luo *et al.* [5] consists of 106 species and 420 reactions. The mechanism was developed using DRG with expert knowledge (DRGX) [39] and DRGASA [33] based on a detailed LLNL mechanism [17]. This mechanism and its variants [10, 11] were coupled to different turbulent combustion models in Spray A flame simulations [8,10-14] and compared with the experimental data from the Engine Combustion Network (ECN). Narayanaswamy *et al.* [40] reduced the improved detailed LLNL mechanism [16] to a skeletal *n*-dodecane mechanism with 255 species and 2289 reactions through multi-stage reduction strategy involving DRGEP [32] and chemical lumping [36]. The reduced mechanism was implemented in a tabulated-chemistry combustion model by Ayyapureddi *et al.* [41] to simulate the Spray A flames. D'Errico *et al.* [42] developed two reduced mechanisms of *n*-dodecane (104 species and 1335 reactions, 88 species and 1158 reactions) using a reduction algorithm combining sensitivity and flux analysis starting from a much smaller detailed mechanism that consists of 435 species and 13,532 reactions. These two mechanisms were also used to simulate the Spray A flames for validation under engine-relevant conditions. These mechanisms are still relatively large and can be expensive for engine simulations, especially when the mechanisms are coupled to advanced combustion models [8, 10, 12,13], or high-fidelity LES studies [14]. More importantly, all of these reduced mechanisms show increased errors in low ambient temperature conditions for Spray A flames, and thus a compact and more accurate mechanism is needed for engine simulations.

In the present work, multiple reduction methods, including RFA and isomer-lumping, are employed to obtain a skeletal mechanism for *n*-dodecane based on a semi-detailed mechanism developed by You *et al.* [43]. The semi-detailed mechanism consists of 171 species and 1306 reactions and has been extensively validated for high temperature (high-T) conditions, which is a good candidate to start with. Semi-global reactions for low-T chemistry are merged to the skeletal mechanism and subsequently optimized to better predict the negative temperature coefficient (NTC) behavior. The final mechanism consists of 54 species and 269 reactions in the skeletal form and is validated against detailed mechanisms and available experimental data. The mechanism is further tuned for and applied in 3-D lifted diesel spray flame simulations.

2. Mechanism development

2.1 Skeletal mechanism development

For a range of conditions in ignition and combustion, the kinetics of fuel decomposition to smaller fragments, which is described by C₅-C₁₂ sub-mechanism, is fast at high-T conditions and can be decoupled from the oxidation kinetics of the H₂ and C₁-C₄ fragments [43]. In the development of the skeletal mechanism, the C₅-C₁₂ sub-mechanism from a detailed mechanism is first simplified by eliminating unimportant species and reactions, and isomer lumping is also employed. The simplified C₅-C₁₂ sub-mechanism is then merged into the simplified H₂/CO/C₁-C₄ base mechanism. Lumped low-T reactions are then added and tuned, resulting in an optimized skeletal mechanism with 54 species and 269 reactions. The reduction and tuning procedure is further discussed in the following.

The detailed C₅-C₁₂ mechanism developed by You *et al.* [43] consists of 60 species and 522 reactions. In the present study, reduction is based on data sampled from homogeneous, adiabatic, isobaric reactors. The parameter range covers pressure of 1–80 bar, equivalence ratio of 0.5–2.0, and initial temperature of 800–1600 K. RFA is first employed to quantify the contribution of each reaction to the generation and consumption of each species. Analysis is conducted from the reactant *n*-dodecane as the starting point. Reaction pathways that are not important to the consumption of *n*-dodecane are removed along with the

species that these paths lead to. Species associated with reaction pathways accumulatively contributing to, for example, 95% of the total consumption of *n*-dodecane are retained. This reduction is performed successively until all the retaining C₅-C₁₂ species find their main pathways to translate into C₁-C₄ fragments. By further applying radical isomers equilibrium assumptions [37], isomers of *n*-dodecyl and other alkyls are lumped to three and one representatives, respectively. The reduced C₅-C₁₂ sub-mechanism obtained after performing species and reactions elimination and isomer lumping consists of 18 species and 60 reactions. It is worth noting that fuel cracking process is fast at high-T conditions during the oxidation of *n*-dodecane and many intermediates are in steady state, only the main reaction pathways that are important for the decomposition of *n*-dodecane to fragments are needed to reproduce this process.

In order to obtain a compact C₀-C₄ sub-mechanism, the C₀-C₄ core in a reduced high-T mechanism for *n*-dodecane oxidation by Vie *et al.* [44] is adopted. This core was reduced from USC-MECH II (111 species and 784 reactions) [45] for high-T oxidation. Two species, namely C₄H₇ and pC₄H₉, and the involved reactions are added to accommodate the C₅-C₁₂ sub-mechanism and more accurately predict the C₄ species concentrations in pyrolysis, which is not considered by Vie *et al.* [44], resulting in a new C₀-C₄ core with 32 species and 191 reactions.

In the end, a semi-global scheme involving 4 species and 18 reactions for low-T chemistry of *n*-decane developed by Bikas and Peters [46] is modified to be suitable for *n*-dodecane and appended to the skeletal mechanism to capture the NTC behavior. Transition between low-T and high-T conditions showing the negative temperature dependence can be well reproduced by applying the Low-T sub-mechanism with lumped reaction steps, which is rather efficient for practical engine simulations [46] and has been fully investigated for *n*-heptane in [47, 48]. A 54-species skeletal mechanism (SK54a) is thereby obtained, which can be found in the supplementary material.

2.2 Need for further tuning

The ignition delay times predicted by SK54a are compared with experimental measurements by Vasu *et al.* [49] and detailed mechanisms [16, 43] in Fig. 1. Simulations are performed under constant-pressure, adiabatic conditions by the SENKIN program [50]. It is seen that the ignition delay times at low-T

conditions ($T < 900$ K) are significantly over-predicted by the You *et al.* mechanism [43] and SK54a while predictions by the LLNL [16] show improved agreement with experimental data.

3-D simulations of Spray A flames are further performed by a three-dimensional computational fluid dynamics code CONVERGE with the experimental flame conditions listed in Table 1. The simulation setup has been reported in our previous studies [12, 51] and will be briefly described here. The Reynolds-averaged Navier-Stokes (RANS) method is used along with the Re-normalization Group (RNG) $k-\epsilon$ turbulence model [52]. The traditional Lagrangian-Eulerian method is employed, where the liquid phase is treated as Lagrangian discrete parcels and the gas-phase is solved on a Eulerian mesh. Source terms are used to exchange mass, momentum, and energy between the two-phases. The “blob” injection method [53] is used with the Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) model [54, 55] for primary and droplet secondary breakup. A dynamic drag model [56] is used to account for the droplet drag. Droplet evaporation is modeled using the Frossling correlation [57]. The gas phase reaction is modeled by a delta function combustion model [58]. The computational region is a cube with dimension of 108 mm in each direction. Adaptive mesh refinement (AMR) is employed to refine the mesh. The minimum cell size is 0.25 mm with peak cell counts in the order of one million. Based on a previous study, this resolution is deemed to be grid convergent for RANS calculations [59]. Ignition delay data measured under a wide range of ambient conditions are used for validation of the newly developed *n*-dodecane skeletal mechanism SK54a. The conditions involve ambient gas temperature of 800-1100 K, fuel injection pressure of 150 MPa, ambient oxygen concentration of (X_{O_2}) 15%, ambient gas density of 22.8 Kg/m³. Ignition delays obtained using SK54a and the previous 106-species mechanism (SK106) [5] are compared with the ECN data [60-62] in Fig. 2 for different ambient temperatures. It is seen that the predictions at 1100 K and 1000 K are better for SK54a mechanism, showing an advantage of SK54a at high-T conditions. At 800 K, SK54a however significantly over-predicts the ignition delay (which is longer than 6 ms and not shown here), showing the need for further tuning of the semi-global low-T reactions.

2.3 Mechanism Tuning

Mechanism tuning is conducted against the detailed LLNL mechanism [16] in auto-ignition, for conditions where experimental data is rare or with large scattering. Simulations are performed under representative conditions of pressure $p = 20$ bar, initial temperature $T_0 = 800$ K and various equivalence ratios as shown in Fig. 3. It is seen that ignition delays are over-predicted by SK54a at lean conditions, while better agreement is observed for rich mixtures. As a result, ignition delay in Spray A flames predicted using SK54a at $T = 800$ K is expected to be longer than that of SK106 which is reduced from LLNL.

Sensitivity analysis is then performed using SK54a at $p = 20$ bar, $\phi = 0.5, 1.0, 2.0$, and $T_0 = 800$ K in the NTC regime to identify the reactions important for low-T ignition. Sensitivity Coefficients (SC) are defined as the resulting percentage change in the ignition delay time (τ) by doubling the rate constant of the i th reaction, k_i [63].

$$SC_i = \frac{\tau(2k_i) - \tau(k_i)}{\tau(k_i)}$$

Eight reactions with the largest magnitude of SC are selected and summarized in Fig. 4. Reactions with positive SC decelerate ignition and make ignition delay longer, and those with negative SC accelerate ignition and result in shorter ignition delay. Sensitivity analysis is also performed under other engine relevant conditions, for example $p = 50$ bar and 80 bar, which shows the same tendency as in $p = 20$ bar and is not showing here.

It can be seen from Fig. 4 that ignition delay under fuel rich condition ($\phi = 2.0$) has larger sensitivity to Low-T reactions (R3, R4, R5) than lean condition ($\phi = 0.5$), which makes it impossible to change ignition delays at lean conditions without affecting rich conditions by tuning these reactions. R1, R2, R6, R7 and R8 are involved in the high-T sub-mechanism and should not be changed. Then it is observed that R1 is more sensitive for lean conditions, for the formation of vinoxy radical (CH_2CHO) facilitates the chain branching of the overall reactivity and the facilitation is more inclined in lean conditions than rich conditions [63]. Although R1 cannot be tuned for its significant influence to high-T oxidation,

decomposition reaction of ketohydroperoxide $\text{OC}_{12}\text{H}_{23}\text{OOH}$ (R9) can be tuned to accelerate CH_2CHO formation which leads to small species through one step reaction ($\text{OC}_{12}\text{H}_{23}\text{OOH} \rightarrow \text{CH}_2\text{O} + 3\text{C}_2\text{H}_4 + \text{C}_2\text{H}_5 + \text{C}_2\text{H}_3\text{CHO} + \text{OH}$). As the products of R9 are selected arbitrarily with reference to Bikas and Peters [46], the $\text{OC}_{12}\text{H}_{23}\text{OOH}$ decomposition reaction is changed to the following formation: $\text{OC}_{12}\text{H}_{23}\text{OOH} \rightarrow 3\text{C}_2\text{H}_4 + \text{C}_2\text{H}_5 + 2\text{CH}_2\text{CHO} + \text{OH}$, to produce vinoxy radicals (CH_2CHO) that can facilitate the chain branching of low-T reactivity. And the rate constant of this reaction is tuned down by a factor of two to accommodate the new mechanism, resulting in the SK54b mechanism, which can be found in the supplementary material. The improved performance of SK54b is shown in Fig. 3.

The tuned mechanism (SK54b) is then employed in 3-D Spray A flame simulations, and predictions of ignition delay are shown in Fig. 5. Over-prediction of ignition delay by ~25% is still observed at the 800 K ambient temperature, which is also observed with SK106 in Fig.2. Since the first stage ignition was found to occur in the lean mixtures and the main ignition in rich mixture [14], ignition delay of the rich case ($\phi = 2.0$) at 800 K is further tuned down by ~25% using another round of reaction tuning based on sensitivity analysis, resulting in the final mechanism (SK54).

More specifically, the second round of sensitivity analysis is performed using SK54b to identify important low-T reactions that are sensitive to ignition delays at $p = 20$ bar, $\phi = 0.5, 1.0, 2.0$ and $T_0 = 800$ K, 900 K. Selected reactions with high sensitivities are shown in Fig. 6. It can be seen that R2 mostly facilitates ignition in all the investigated cases as indicated by the negative sensitivity coefficients. R6 accelerates ignition of fuel rich conditions and decelerates ignition of fuel lean conditions at $T_0 = 800$ K, which however has little effect on the ignition delays at $T_0 = 900$ K. Therefore, tuning up rate constants of R2 and R6 will result in a further decrease of ignition delay at $\phi = 2.0$, $T_0 = 800$ K and ignition delays at $T_0 = 900$ K and $\phi = 0.5$, $T = 800$ K are mostly unchanged. The tuning of these two reactions (R2 and R6) is conducted through careful trial and error iterations, leading to the final mechanism (SK54), which can be found in the supplementary material. Performance of SK54 after this round of tuning is shown in Fig. 5. It is seen that the ignition delay time at $T_0 = 800$ K is better predicted by SK54.

3. Mechanism Validation

3.1 Validation for elementary reactors and flames

The mechanism is first validated for shock tube ignition delay data [49,64] at various pressures and equivalence ratios. Fig. 7 shows comparison between experimental data and predicted ignition delays for pressure of 20 bar and 50 bar, and various equivalence ratios. It is seen that the present mechanism agrees well with the experimental data, and the overall discrepancy is smaller than that using the detailed LLNL mechanism due to the tuning of low-T chemistry. It is therefore expected that the auto-ignition delays of homogeneous mixtures can be more accurately captured for flames that fall within the above parameter range, which is relevant to the Spray A flame conditions.

To further verify the performance of the mechanisms, especially the simplified C₅-C₁₂ fuel cracking sub-mechanism, pyrolysis of *n*-dodecane in perfectly stirred reactors (PSR) [65] and flow reactors [66] is simulated with the present mechanism and compared with the experimental data by Herbinet *et al.* [67] and Dahm *et al.* [68]. Fig. 8 shows the comparison of the *n*-dodecane conversion rate calculated with different mechanisms [16, 43] in comparison with experimental data. Species profiles during the pyrolysis processes are further compared in Figs. 9-10. It is seen that the reduced mechanism shows overall similar accuracy in the different pyrolysis cases to that of the more detailed You *et al.* mechanism, for these two mechanisms share the high-T chemistry, while the LLNL mechanism shows overall larger discrepancies.

Figure 11 shows species profiles of *n*-dodecane oxidation in PSR predicted by SK54 compared with the experimental data by Mzéahmed *et al.* [18]. Predictions above 700 K agree well with experimental data, while some discrepancies exist at temperatures lower than 700 K. The NTC behaviors are under-predicted by the present mechanism at T = 650 K, while the overall agreement is still reasonable.

Figure 12 shows extended validations of the laminar flame speeds of *n*-dodecane/air mixtures during one-dimensional (1-D) flame simulations [69] evaluated using SK54 and You *et al.* mechanism [43], in comparison with experimental data in literature [70-72]. Agreement between SK54 and You *et al.*

mechanism is of the order of the scatter of the experimental data at various conditions of pressures, inlet temperatures and equivalence ratios. This is expected since the flame speeds are primarily controlled by high-T chemistry, while You *et al.* mechanism and SK54 share the C₀-C₄ core, which has been extensively validated against flame speeds data, although some discrepancy exists for the simplification. Also, the present skeletal mechanism is primarily developed for simulations of diesel engine relevant conditions for which absolutely accurate prediction of laminar flame speeds is not so necessary [5].

3.2 Validation for 3-D spray flame simulations

The newly developed skeletal mechanism SK54 is further applied to simulate spray flames. The simulation results are compared with experimental data performed under compression-ignition (CI) engine conditions from the ECN [60,73-75]. The experimental and computational configurations are shown in Table 1. Details of the 3D simulations have been described in section 2.2.

Figure 13 shows the comparison of experimental data and predicted ignition delay and Lift-off length (LOL) at fuel injection pressure of 150 MPa, ambient oxygen concentration of (XO₂) 15%, ambient gas density of 22.8 Kg/m³ and various ambient temperatures. It is seen from Fig. 13a that the ignition delays are well reproduced at high-T conditions (T > 1000 K), indicating the high fidelity of the high-T sub-mechanism in the skeletal mechanism. Some discrepancies are observed at low-T conditions wherein ignition delays are under-predicted at ambient temperatures of 900 K and 850 K, and slightly over-predicted at 800 K. The differences may be due to the simplification of the lumped low-T oxidation sub-mechanism. It is noted that the prediction at 800 K is within the experimental uncertainty range. The LOL comparison is reported in Fig. 13b. It is seen that the present mechanism accurately reproduces the experimental LOL data at both low and high-T conditions. Overall, the predictions of the present mechanism are reasonably good compared to the measurements for the wide range of ambient temperatures investigated.

Figures 14 and 15 show the comparisons of ignition delay and LOL between the experimental data and predictions at ambient gas temperature of 900 K, ambient gas density of 22.8 Kg/m³, different fuel

1 injection pressures and ambient oxygen concentrations. Overall, the simulations capture the experimental
2 trends well. As the present mechanism under-predicts ignition delays at the condition $T=900$ K, all cases
3 in Fig. 14a show about 10-20% shorter ignition delays compared to the experimental data. Similar
4 observation is made in Fig. 15a also at different oxygen concentrations. However, the predictions of LOL
5 presented in Figs. 14b and 15b are in good agreement with experiments.

6 Comparisons of ignition delay and LOL at ambient gas temperature of 900 K, fuel injection pressure
7 of 150 MPa, ambient oxygen concentration of (X_{O_2}) 15% and different ambient densities are shown in
8 Fig. 16. Again, the ignition delays are under-predicted with larger discrepancies at lower ambient
9 densities. Overall, the ignition delays and LOL at these ambient densities are reasonably reproduced by
10 the skeletal kinetic mechanism.

11 **4. Conclusions**

12 A compact skeletal mechanism with 54 species and 269 reactions is developed for *n*-dodecane using a
13 hybrid and decoupling approach. High-T C_5 - C_{12} sub-mechanism is firstly simplified from the detailed
14 mechanism of You *et al.* [43] by eliminating species and reactions guided by RFA and isomer lumping.
15 The C_5 - C_{12} reduced sub-mechanism is then merged to a reduced C_0 - C_4 core based on the USC-Mech II
16 [45]. Semi-global reactions for NTC chemistry are added and tuned against the detailed LLNL
17 mechanism [16] and experimental data to eventually obtain a 54-species skeletal mechanism SK54.

18 The skeletal mechanism SK54 is validated against experimental data for shock tubes, PSR, flow
19 reactors, and laminar flame speeds, and compared with other mechanisms. It is shown that the skeletal
20 mechanism performs well over a wide range of parameters in elementary flame experiments.
21 Furthermore, the skeletal mechanism was applied for 3-D Spray A flame simulations. Comparison with
22 experimental data obtained from the ECN shows that the ignition delays and flame LOL are reasonably
23 well reproduced by the tuned skeletal mechanism under various conditions, thus providing a valid option
24 for efficient and accurate multi-dimensional engine combustion simulations.

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15 **6. Supplementary material**

16 Supplementary data including newly developed mechanisms (SK54a, SK54b, SK54) associated with
17 this article can be accessed on online.

18 **7. References**

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Table captions:

Table 1. Experimental configuration of Spray A from the ECN [60-62]

Tables:

Table 1.	
Parameter	Quantity
Fuel	<i>n</i> -dodecane
Nozzle outlet diameter	90 μm
Discharge coefficient	0.86
Fuel injection pressure	50 - 150 MPa
Injection duration	1.5 ms
Ambient gas temperature	800 – 1200 K
Ambient gas density	7.6 - 22.8 kg/m ³
Ambient oxygen	13 - 21%

Figure Captions

Fig. 1. Comparison of experimental [49] and calculated constant-pressure auto-ignition delay times as function of temperature using SK54a, You *et al.*[43], and the detailed LLNL mechanism [16] for *n*-dodecane/air mixtures at $p = 20$ bar and $\phi = 0.5$ and 1.0 .

Fig. 2. Ignition delay in 3-D Spray A simulations using SK54a and SK106, in comparison with experimental data [60-62].

Fig.3. Ignition delay as function of equivalence ratio calculated using SK54a, SK54b and the detailed LLNL mechanism [16] for *n*-dodecane/air mixture at $p = 20$ bar and $T_0 = 800$ K.

Fig. 4. Selected reactions with high sensitivities for constant-pressure ignition delay of *n*-dodecane/air at $p = 20$ bar, $T_0 = 800$ K, and $\phi = 0.5, 1.0, 2.0$, calculated using SK54a.

Fig. 5. Ignition delay in 3-D Spray A simulations using SK54a, SK54b and SK54 in comparison with experimental data [60-62].

Fig. 6. Selected reactions with high sensitivities for constant-pressure ignition delay of *n*-dodecane/air calculated using SK54b at $p = 20$ bar, $\phi = 0.5, 1.0, 2.0$ and different initial temperatures (a) $T_0 = 800$ K, (b) $T_0 = 900$ K.

Fig. 7. Ignition delay as function of temperature calculated using SK54 and the detailed LLNL mechanism [16], respectively, in comparison with shock tube experimental data [49, 64] for *n*-dodecane/air mixtures at different pressures and equivalence ratios.

Fig. 8. Calculated versus experimentally measured [65, 66] fuel consumption rates as function of residence time in a) jet stirred reactors at $T = 873$ K and 973 K, $p = 1$ atm, for 2% (mole) *n*-dodecane in He, and b) flow reactors at $T = 950$ K, 1000 K and 1050 K, $p = 1$ atm, for 0.336% (mole) *n*-dodecane in N_2 .

Fig. 9. Species concentrations as function of residence time calculated using different mechanisms in comparison with experimental data [65] for jet stirred reactors at $T = 973$ K, $p = 1$ atm, for 2% (mole) *n*-dodecane in He.

Fig. 10. Species concentrations as function of residence time calculated using different mechanisms in comparison with experimental data [66] for flow reactors at $T = 1050$ K, $p = 1$ atm for *n*-dodecane.

Fig. 11. Comparison of calculated and measured *n*-dodecane oxidation species profiles in JSR, at $p = 10$ bar, $\tau = 1$ s, and different equivalence ratios (a) $\phi = 1.0$, (b) $\phi = 2.0$, for 0.1% (mole) *n*-dodecane in O_2 and N_2 . Lines: simulation results using SK54, symbols: experimental data [18].

Fig. 12. Laminar flame speeds for *n*-dodecane/air mixtures at different inlet temperatures, pressures and equivalence ratios, calculated using different mechanisms in comparison with experimental data [70-72].

Fig. 13. Measured [60, 73-75] and predicted ignition delay and LOL as function of ambient temperature. The error bar shows the experimental uncertainty.

Fig. 14. Measured [60, 73-75] and predicted ignition delay and LOL as function of injection pressure. The error bar shows the experimental uncertainty.

Fig. 15. Measured [60, 73-75] and predicted ignition delay and LOL as function of ambient oxygen concentration. The error bar shows the experimental uncertainty.

Fig. 16. Measured [60, 73-75] and predicted ignition delay and LOL as function of ambient gas density. The error bar shows the experimental uncertainty.

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