



On lumped-reduced reaction model for combustion of liquid fuels



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ABSTRACT

A systematic approach to developing compact reduced reaction models is proposed for liquid hydrocarbon fuels using *n*-dodecane and *n*-butane as the model fuels. The approach has three elements. Fast fuel cracking reactions are treated by the quasi-steady state approximation (QSSA) and lumped into semi-global reactions to yield key cracking products that are C_1 – C_4 in size. Directed relation graph (DRG) and sensitivity analysis reduce the foundational fuel chemistry model to a skeletal model describing the oxidation of the C_1 – C_4 compounds. Timescale-based reduction using, e.g., QSSA, is then employed to produce the final reduced model. For *n*-dodecane, a 24-species reduced model is derived from JetSurF and tested against the detailed model for auto-ignition, perfectly stirred reactors (PSR), premixed flame propagation, and extinction of premixed and non-premixed counterflow flames. It is shown that the QSSA of fuel cracking reactions is valid and robust under high-temperature conditions from laminar flames, where mixing is controlled by molecular diffusion, to perfectly stirred reactors, which correspond to the limit of fast turbulent mixing. Bifurcation analysis identifies the controlling processes of ignition and extinction and shows that these phenomena are insensitive to the details of fuel cracking. To verify the applicability of the above finding to turbulent flames, 2-D direct numerical simulation (DNS) of a lean turbulent premixed flame of *n*-butane/air with Karlovitz number of 250 was carried out using a reduced model developed from USC-Mech II. The results show that QSSA for fuel cracking remains valid even under intense turbulence conditions. Statistical analysis of the DNS data shows that fuel cracking is complete before the flame zone, and for the conditions tested, turbulent transport does not bring any significant fuel molecules into the flame zones, thus further substantiating the validity of the approach proposed.

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1. Introduction

Practical engine fuels typically contain a large number of components with wide varying molecular structures. In addition to the multicomponent nature, the high complexity of practical fuel combustion chemistry is also attributed to the myriad intermediate species generated during the pyrolysis and oxidation processes. While developments employing detailed modeling and surrogate fuel approaches are advancing rapidly, challenges abound in the application of the chemistry model in turbulent flame simulations. Both the underlying chemical complexities, which lead to model inaccuracy, and the large model size, which imposes infeasible computational expense, are some of the fundamental factors that limit the broader utilization of the chemistry efforts.

Fuel cracking is slow and rate-limiting at low-temperature conditions, and thus typically needs to be resolved [1–3]. However, fuel cracking through beta-scission occurs rather fast at high temperatures compared to the subsequent oxidation of the resulting small molecules. In a previous work, You et al. [4] examined the reaction chemistry of *n*-dodecane combustion under a wide range of conditions. The primary conclusion of that study is that in high-temperature (high-T) combustion, *n*-dodecane undergoes complete pyrolysis, yielding methane, ethylene, propene, butene, and molecular hydrogen, before these smaller molecular weight fragments are oxidized. The oxidation of these fragments is rate-limiting for all conditions tested. These conclusions are consistent with experimental observations made later in shock tubes [5,6]. For these reasons, the fuel cracking processes may be approximated by a few semi-global reaction steps [4], which can subsequently be grafted on to a detailed C_1 – C_4 model core, e.g., the USC-Mech II [7], to obtain compact hybrid models for high-T combustion [4,8]. The resulting models can further be reduced [9]. For instance, a 24-species reduced model was

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Table 1
The skeletal fuel pyrolysis sub-model for *n*-dodecane.

No.	Reaction	<i>A</i>	<i>n</i>	<i>E_a</i>
1	$n\text{-C}_{12}\text{H}_{26} \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_2\text{H}_4 + n\text{-C}_3\text{H}_7 + \text{CH}_3$	8.53×10^{23}	-2.03	90,034
2	$n\text{-C}_{12}\text{H}_{26} \Rightarrow \text{C}_6\text{H}_{12} + 2n\text{-C}_3\text{H}_7$	5.64×10^{26}	-2.68	88,171
3	$n\text{-C}_{12}\text{H}_{26} \Rightarrow \text{C}_4\text{H}_8\text{-1} + \text{C}_2\text{H}_4 + 2n\text{-C}_3\text{H}_7$	7.88×10^{25}	-2.65	88,391
4	$n\text{-C}_{12}\text{H}_{26} \Rightarrow 2\text{C}_3\text{H}_6 + 2n\text{-C}_3\text{H}_7$	4.00×10^{26}	-2.66	88,392
5	$n\text{-C}_{12}\text{H}_{26} + \text{H} \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{H}_2$	1.30×10^6	2.54	6756
6	$n\text{-C}_{12}\text{H}_{26} + \text{H} \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{H}_2$	5.20×10^6	2.40	4471
7	$n\text{-C}_{12}\text{H}_{26} + \text{O} \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{OH}$	2.50×10^6	2.40	5504
8	$n\text{-C}_{12}\text{H}_{26} + \text{O} \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{OH}$	4.60×10^5	2.60	1768
9	$n\text{-C}_{12}\text{H}_{26} + \text{OH} \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{H}_2\text{O}$	1.40×10^7	1.80	974
10	$n\text{-C}_{12}\text{H}_{26} + \text{OH} \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{H}_2\text{O}$	4.00×10^6	2.00	-596
11	$n\text{-C}_{12}\text{H}_{26} + \text{CH}_3 \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{CH}_4$	9.03×10^{-1}	3.65	7153
12	$n\text{-C}_{12}\text{H}_{26} + \text{CH}_3 \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{CH}_4$	6.00	3.46	5480
13	$n\text{-C}_{12}\text{H}_{26} + \text{O}_2 \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{HO}_2$	4.00×10^{13}	0.00	50,930
14	$n\text{-C}_{12}\text{H}_{26} + \text{O}_2 \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{HO}_2$	1.60×10^{14}	0.00	47,590
15	$n\text{-C}_{12}\text{H}_{26} + \text{HO}_2 \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{H}_2\text{O}_2$	4.76×10^4	2.55	16,490
16	$n\text{-C}_{12}\text{H}_{26} + \text{HO}_2 \Rightarrow \text{C}_6\text{H}_{12} + \text{C}_3\text{H}_6 + n\text{-C}_3\text{H}_7 + \text{H}_2\text{O}_2$	3.80×10^4	2.60	13,910

Note: Rate coefficient expressed as $k = AT^n \exp(-E_a/RT)$. Units are mole, cm, s, cal, and K.

developed from a version of JetSurF with lumped fuel cracking reaction steps [8] using directed relation graph (DRG) [9–11], DRG aided sensitivity analysis (DRGASA) [12,13], and linearized quasi-steady state approximations (LQSSA) [14], and was applied in direct numerical simulations (DNS) of a turbulent counterflow *n*-dodecane spray flame [15].

Nevertheless, in the work of You et al. [4], most of the combustion properties considered are those with negligible back mixing of burned or unburned mixtures. What was also not adequately studied was the near-limit phenomena, notably the extinction and ignition states in perfectly stirred reactors (PSR), which are typically turning points of the *S*-curve response [16]. In the present study, we investigate the potential of using combined hybrid model development and model reduction to obtain highly efficient reduced models with less than 30 species for large hydrocarbon fuel combustion at high-T conditions. First, this hybrid model is assessed using the 24-species reduced model for *n*-dodecane and a variety of reactors and flames, including auto-ignition, PSR, premixed flame propagation, and extinction of premixed and non-premixed counterflow flames. The validity of the assumption of fast fuel cracking at high temperature conditions is subsequently investigated with 2-D DNS of a lean turbulent premixed flame for *n*-butane/air using a reduced model derived from the detailed USC-Mech II.

2. Performance of a reduced model for *n*-dodecane with lumped fuel cracking steps

2.1. A brief review of the reduced model

An approach to lump the fuel cracking reactions has been demonstrated in [4,8]. This approach assumes that the intermediates of the fuel cracking are all in quasi-steady state. It reduces the chemical complexity of the reaction processes and the model size in an efficient manner. For *n*-dodecane, the resulting lumped model contains only three species, namely, *n*-dodecane, 1-pentene and 1-hexene and approximately one and a half dozen reactions. The rate coefficients of the lumped reaction model are based on JetSurF 1.0 [17]. The lumped pyrolysis model was combined with USC-Mech II [7] to obtain a complete model of 123 species and 977 reactions, referred to as JetSurF 1.0-1, which has been validated against the detailed model and experiments over a wide range of conditions [8]. Subsequently, this lumped-detailed reaction model was reduced to 24 species and employed in a study of spray combustion of *n*-dodecane in a turbulent counterflow flame [15].

The three steps taken in the above model reduction are described here. The DRG-based methods, including DRG and DRGASA, were

employed to remove unimportant species and reactions first from a range of combustion responses over the pressure range of 1 to 10 atm, initial temperatures from 1000 to 1600 K for auto-ignition, inlet temperature of 300 K for PSRs, and equivalence ratios from 0.5 to 1.5. The H atom was selected as the starting species in the graph searching in DRG and the obtained skeletal model consists of 47 species and 359 reactions. After skeletal reduction with DRG, the model was further reduced with DRGASA to obtain a smaller model. The worst case error in target parameters induced by removing a single species was first tested and then sorted in ascending order. The species were then eliminated one by one until the worst case error in the target parameters reaches the given error tolerance. In DRGASA, auto-ignition delay with initial temperature from 1000 to 1600 K and extinction residence time of PSRs with inlet temperature of 300 K over the pressure range of 1 to 10 atm and equivalence ratio from 0.5 to 1.5, were selected as the target responses with an error tolerance of 20%. The final skeletal model is comprised of 193 reactions and 31 species: N₂, H, O, OH, HO₂, H₂, H₂O, H₂O₂, O₂, CH₂, CH₂^{*}, CH₃, CH₄, HCO, CH₂O, CH₃O, CO, CO₂, C₂H₂, C₂H₃, C₂H₄, C₂H₅, C₂H₆, CH₂CHO, aC₃H₅ (allyl), C₃H₆, *n*C₃H₇, C₂H₃CHO, C₄H₈-1 (1-butene), *n*C₁₂H₂₆ (*n*-dodecane), and C₆H₁₂ (1-hexene). Reactions of any eliminated species were also removed. The skeletal sub-model for fuel pyrolysis is provided in Table 1. In the last step, this skeletal model was further reduced with the LQSSA method [14]. Seven global QSS species, namely CH₂, CH₂^{*}, HCO, CH₃O, C₂H₃, C₂H₅, and *n*C₃H₇, were identified by excluding all species with nontrivial projection to the slow chemical subspace, thus resulting in a 24-species model. The QSS species are eliminated from the transport equations and can be solved with a set of internal algebraic equations. The QSSA equations are evaluated analytically using a graph-based method [14] to ensure high accuracy and robustness.

2.2. Extended model validation

Validation of the reduced model is rather limited in Ref. [15] and is extended in the present study, particularly regarding the effects of fuel cracking. The reduced model is first compared with the detailed JetSurF 1.0 and the lumped-detailed model, in which the elementary fuel cracking reactions of JetSurF 1.0 are replaced by lumped semi-global steps, for ignition delay and PSR extinction over a wide range of pressures, temperatures and equivalence ratios. Figure 1 shows excellent agreement of the three models despite some minor discrepancies between the detailed and lumped-detailed models.

The normalized total mass fraction of the species with four or more carbon atoms, denoted by C₄₊, are plotted in Fig. 2 as a function of temperature in auto-ignition and PSRs for different equivalence

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