Chinese Journal of Chemical Engineering 56 (2023) 225–232

Contents lists available at ScienceDirect

Chinese Journal of Chemical Engineering

journal homepage: www.elsevier.com/locate/CJChE

Full Length Article

Theoretical and experimental study on the inhibition of jet fuel oxidation by diarylamine

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ARTICLE INFO

Article history:
Received 21 July 2022
Received in revised form 6 September 2022
Accepted 25 September 2022
Available online 28 October 2022

Keywords:
Jet fuel
Thermal oxidation stability
High-energy–density fuel
Diarylamine
Antioxidation mechanism

ABSTRACT

Antioxidants addition is believed as a facile and effective way to improve jet fuel thermal oxidation stability. However, amine antioxidants, as one of the most important antioxidants, have not received sufficient attention in the field of jet fuel autoxidation yet. Herein, the inhibition efficiency and mechanism of decane and *exo*-tetrahydrodicyclopentadiene (THDCPD) oxidation by di-4-*tert*-butylphenylamine (diarylamine) was experimentally and theoretically investigated. The results show that diarylamine can significantly inhibit decane oxidation but is less efficient for THDCPD oxidation, which is attributed to the higher energy barrier of retro-carbonyl-ene reaction (rate-determining step) in THDCPD than that in decane during diarylamine regeneration. However, the addition of diarylamine will cause undesirable color change after accelerated oxidation and produce slightly more deposits during high-temperature thermal oxidative stress for both decane and THDCPD. The results provide significant implications for the future design of effective antioxidant additives for high-performance jet fuel.

1. Introduction

Besides the primary use for propulsion *via* combustion, jet fuel plays an important role as a coolant for cooling hot subsystems in current high-performance aircrafts [1,2]. When jet fuel is used as a coolant in advanced engines, it will experience oxidative deterioration and produce thermal oxidative deposits (originated from fuel oxidation) in severe case. Therefore, it is imperative to prevent fuel oxidative deterioration and deposition. To date, a variety of approaches have been developed to prevent oxidative deterioration, of which several feasible methods are as follows: fuel deoxygenation to remove dissolved oxygen [3,4], fuel processing to remove unstable component (*e.g.*, heteroatomic compounds or dissolved metal) [5] and antioxidants addition [6,7]. Among them, the antioxidants addition is the most facile and effective way [7,8]. Two main classes of antioxidants are phenols and amines, and both have been widely utilized to protect a variety of chemical products, such as medicine, food, polymeric materials, and so on [9–11]. For example, Borsato *et al.* [12] observed that the addition of the synthetic phenolic antioxidants, butylhydroxyanisole (BHA), *tert*-butyl-hydroquinone (TBHQ) and butylated hydroxytoluene (BHT) or their blends, can significantly inhibit the oxidation of biodiesel from soybean. Our previous study also demonstrated that the addition of phenolic antioxidants can inhibit fuel oxidation and prolong the shelf life, and the antioxidants that can scavenge more radicals per molecule will show better performance [7].

Recently, amine antioxidants have attracted significant attention because of their high antioxidation activity and efficiency at high temperatures [13]. Among the amine antioxidants, diphenylamines are the most widely used radical trapping antioxidants. Analogous to phenolic antioxidants, diphenylamines will initially donate the aminic H-atom to peroxyl radicals (Eq. (1), where Ar represents the aromatic ring) [14]. Subsequently, the consequent aminyl radical will react with another peroxyl radical leading to nonradical products at ambient temperature (Eq. (2)) or nitroxide radical at elevated temperature (especially > 120 °C, Eq. (3)). The latter reaction is the key to the high antioxidation activity of diphenylamines since they can be regenerated *via* the unique

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https://doi.org/10.1016/j.cjche.2022.09.015
1004-9541/

catalytic antioxidation mechanism [15]. In this case, the stoichiometric factors, defined as the number of active radicals scavenged by one antioxidant molecule, can sharply increase to 41 for the inhibited autoxidation of paraffin oil at 130 °C (the stoichiometric factor of phenol is only 2) [16]. Based on the above mechanism, the development of novel diphenylamine with much higher antioxidation efficiency is constantly increasing [17–19]. For example, Hanthorn *et al.* [20] designed a compound with outstanding reactivity toward peroxyl radicals (radical-trapping activities up to 200-fold greater than those of typical commercial diphenylamines) by the incorporation of nitrogen atoms into the aromatic rings of diphenylamine. Besides the high antioxidation efficiency of diphenylamine, the regeneration feature may also be conducive to mitigating fuel thermal oxidative deposition since the oxidation products of both jet fuel and diphenylamine, which are precursors of deposits, can probably be avoided. However, the applicability of diphenylamine in commercial jet fuel has not yet been demonstrated. According to the ASTM D7566, only three sterically hindered phenols, namely 2,6-ditertiary-butyl phenol, 2,6-ditertiary-butyl-4-methyl phenol, and 2,4-dimethyl-6-*tert*-butyl-phenol or their mixtures are applicable for preventing the oxidation and the formation of polymeric oxidation products during jet fuel storage and/or usage [21].

$$Ar_2NH + ROO\cdot \rightarrow Ar_2N\cdot + ROOH \quad (1)$$

$$Ar_2N\cdot + ROO\cdot \rightarrow \text{nonradical products} \quad (2)$$

$$Ar_2N\cdot + ROO\cdot \rightarrow Ar_2NO\cdot + RO\cdot \quad (3)$$

More recently, the high-energy–density fuel (HED fuel) has drawn significant attention, because compared with conventional kerosene-based fuel, it can provide more propulsion energy to extend the flight range and/or increase the payload of volume-limited aircraft [22,23]. To ensure the high energy density, HED fuel is normally composed of multi-cyclic hydrocarbons [24], however, according to our previous study, the multi-cyclic hydrocarbons, such as *trans*-decalin and *exo*-tetrahydrodicyclopentadiene, exhibit inferior thermal oxidation stability [25]. Improving the thermal oxidation stability of HED fuel by introducing antioxidants will be highly attractive as it can simultaneously promote the aircraft performances of long flight distance and high speed [26,27], and diphenylamine seems to be a promising candidate as it has high antioxidation activity at elevated temperature.

Herein, the inhibition of diarylamine toward the oxidation of two different kinds of jet fuels (conventional kerosene-based fuel and HED fuel) were investigated theoretically and experimentally. The decane was chosen to represent conventional kerosene-based fuel and *exo*-tetrahydrodicyclopentadiene (THDCPD) was chosen as HED fuel since it is the main component of typical JP-10 HED fuel (with the density of 0.94 $g\cdot cm^{-3}$ at 15 °C and the volumetric net heat of combustion of 39.6 $MJ\cdot L^{-1}$) [22,28]. Considering the solubility of diarylamine in jet fuel, the di-4-*tert*-butylphenylamine (abbreviated as diarylamine below) with two nonpolar tertiary-butyl groups at *para* positions was adapted. The results reveal that diarylamine can effectively delay oxidation and prolong the shelf time of decane but present inferior performance in delaying THDCPD oxidation. Importantly, the addition of diarylamine cannot mitigate the thermal oxidative deposits for both decane and THDCPD when they serve as the coolant but will cause slightly more deposits.

2. Materials and Methods

2.1. Computational details

All density functional theory (DFT) calculations were performed using the hybrid B3LYP functional with the Gaussian 03 program package [29,30]. The 6-311G(d,p) basis set was used to optimize structures and for subsequent frequency calculations to characterize stationary points as minima or first-order saddle points. According to previous study [31,32], B3LYP has been proven to provide energies close to more sophisticated and time-consuming methods for related systems. Geometry optimizations were confirmed as local minima by the absence of imaginary frequencies in the vibrational spectra. Transition states were optimized using the QST3 method as implemented in Gaussian software. The transition state structures were confirmed *via* the presence of a single imaginary frequency corresponding to the saddle point. Intrinsic reaction coordinate (IRC) calculations were also performed to verify that the identified products and the reactants were correctly connected [33]. For radicals and transition states (open-shell systems), unrestricted DFT calculations were carried out and the results obtained were checked for wave function instability, and restricted calculations were performed on closed-shell (stable) species [34]. All the enthalpy values were obtained as a sum of electronic and thermal correction to the total electronic energies.

2.2. Experimental procedures

Normal decane (with the purity >99.5 wt.%) used in this study was supplied by Macklin Co. Ltd, and THDCPD with the purity of 99.5 wt.% (by GC) was synthesized according to our previous work [35]. The pristine fuel samples did not contain any antioxidant additives. Di-4-*tert*-butylphenylamine (analytical grade) was purchased from Shanghai Aladdin Industrial Corporation and added to the fuel samples at the concentrations of 0.1, 0.5, 1.0, 1.5, 2.0, and 2.5 $mmol\cdot L^{-1}$, after which the treated fuel samples were kept at room temperature in the dark to avoid the autoxidation during the storage.

According to the references and our previous study [7,25,36], the rapid small scale oxidation tester (RSSOT, specified in the ASTM D7545) is suitable for studying jet fuel autoxidation, and thus the efficiency of diarylamine in antioxidation of decane and THDCPD was evaluated by Rapid Oxy device (Anton Paar, Dahlewitz, Germany). Typically, 5 ml of fuel sample with different concentrations of diarylamine was introduced into the hermetically sealed test chamber. After being purged by pure oxygen, the reaction chamber was pressured to 700 kPa and then heated to 140 °C. The oxygen pressure was monitored continuously throughout the accelerating oxidation process. The pressure drop is correlated with oxygen consumption, and the induction period (IP) refers to the time when 10% pressure drop of the recorded highest pressure occurs (Fig. 1), which can be correlated with fuel oxidation stability [7,37]. The oxidation stability of jet fuels is more relevant to their long-term storage stability, and normally the higher oxidation stability refers to longer shelf life.

The thermal oxidative deposition of jet fuels is more crucial to their practical application when used as the coolant, and thus the jet fuel thermal oxidation stability tester (JFTOT) was adopted for assessing the effect of diarylamine on jet fuel thermal oxidative deposition in this work according to the ASTM D3241 [5,27,38]. Briefly, 960 ml fuel sample is initially filtrated through a single layer filter and followed by aeration for 6 min at 1.5 $L\cdot min^{-1}$ air flow rate using a borosilicate gas dispersion tube to saturate the fuel sample with dissolved oxygen (*ca.* 70 $mg\cdot L^{-1}$). Subsequently, the fuel is pressured to 3.45 MPa and pumped at a volumetric flow rate of 3 $ml\cdot min^{-1}$ through the hot test tube at the set temperature

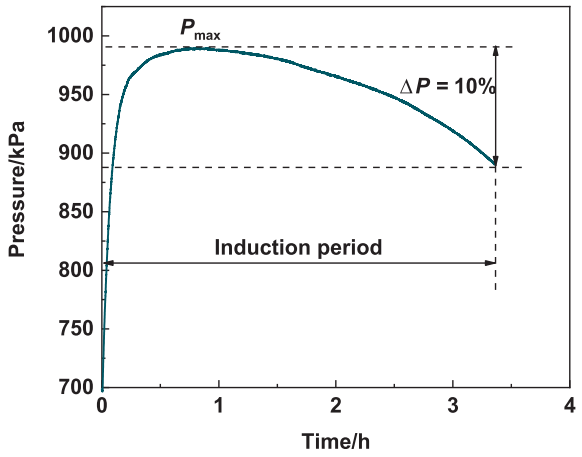

Fig. 1. Definition of induction period of pristine decane in Rapid Oxy device.

Table 1
Test conditions in JFTOT

Parameters	Values
Temperature/°C	355
Fuel volume/ml	960
Fuel flow rate/ml·min^{-1}	3
Fuel pressure/MPa	3.45
Test time/h	5
Aeration time/min	6
Air flow rate/L·min^{-1}	1.5

and the color change of the test tube caused by thermal oxidative deposits can occur, after which the fuel enters a precision stainless steel filter where the oxidative degradation (insoluble) products (>17 μm) in the bulk fuel may be trapped. Table 1 summarizes the detailed test conditions in JFTOT. The tested tubes were initially evaluated qualitatively by visual tube rater (VTR) to access the pass/fail result. After that, the ellipsometric tube rater (ETR) was further adopted to quantitatively access the thickness of surface deposit of the tested tubes. To prove the repeatability and evaluate the uncertainty, each evaluation was performed for at least twice.

3. Results and Discussion

3.1. Molecular modeling

It is widely accepted that the formation of hydroperoxide *via* the hydrogen abstraction by peroxyl radical from hydrocarbon molecular is the rate-determining step of jet fuel autoxidation [39–41]. In many respects closely behaving as phenols, diphenylamines prefer to donate the aminic H-atom to peroxyl radicals rather than the hydrocarbon molecular. In this case, the N—H bond dissociation energy (BDE) should be the main factor affecting its efficiency. The calculated N—H BDE of diphenylamine is only 364.9 kJ·mol^{-1}, which is much lower than the lowest C—H BDE of decane (438.6 kJ·mol^{-1}) and THDCPD (433.2 kJ·mol^{-1}). To further elucidate the antioxidation activity of diphenylamine, the activation energy of hydrogen abstraction was calculated. The results in Fig. 2 reveal that the hydrogen abstraction of decane and THDCPD requires relatively high energy barriers of 88.5 kJ·mol^{-1} and 86.2 kJ·mol^{-1}, respectively. However, from Fig. 3(a), the energy barriers of hydrogen abstraction from diphenylamine to hydrocarbon are only 19.0 kJ·mol^{-1} (for decane) and 11.0 kJ·mol^{-1} (for THDCPD), respectively, with the calculated TS structures for the reaction between diarylamine and peroxyl radicals shown in Fig. 4. These results indicate that diphenylamine is inclined to donate H-atom to stabilize the peroxyl radical to give a hydroperoxide and a diarylaminyl radical. Therefore, diphenylamine has antioxidation effects on decane and THDCPD.

However, different from phenolic antioxidants, diphenylamine will be regenerated during antioxidation. Fig. 3(b) shows the regeneration mechanism of diphenylamine [14], and the structures and energetics of the compounds in the proposed regeneration mechanism of diphenylamine were further calculated by DFT. As shown in Fig. 3(b), the resultant diarylaminyl radical after hydrogen abstraction will further couple to a peroxyl radical to yield an alkoxyamine. The results presented in Fig. 3 show that the coupling of diarylaminyl radical to peroxyl radicals is exothermic (101.1 kJ·mol^{-1} for decane and 105.4 kJ·mol^{-1} for THDCPD) and expected to be diffusion-controlled. Actually, side reactions can also occur in this step. For example, the diarylaminyl radical may rearrange into phenoxyl radicals, and then the peroxyl radical will couple with the phenoxyl radical at aryl ring, which may rapidly consume the diphenylamine and significantly reduce its stoichiometric factor [14,42]. Subsequently, the formed alklperoxyamine can cleave alkoxy to yield diphenylnitroxide, which can combine with an alkyl radical to afford alkoxyamine. The combination of an alkyl radical to the diphenylnitroxide is also exothermic (188.9 kJ·mol^{-1} for decane and 182.2 kJ·mol^{-1} for THDCPD).

Then, the alkoxyamine will undergo a six-electron retro-carbonyl-ene pericyclic process (or in-cage disproportionation), which would give the same carbonyl product and an imino-tautomer of diphenylamine. Fig. 5 shows the optimized transition state structures for the retro-carbonyl-ene reaction, and the calculated energy barrier of this process is 142.9 kJ·mol^{-1} for decane and 149.7 kJ·mol^{-1} for THDCPD, respectively, which is much higher than that of hydrogen abstraction, making it the rate-

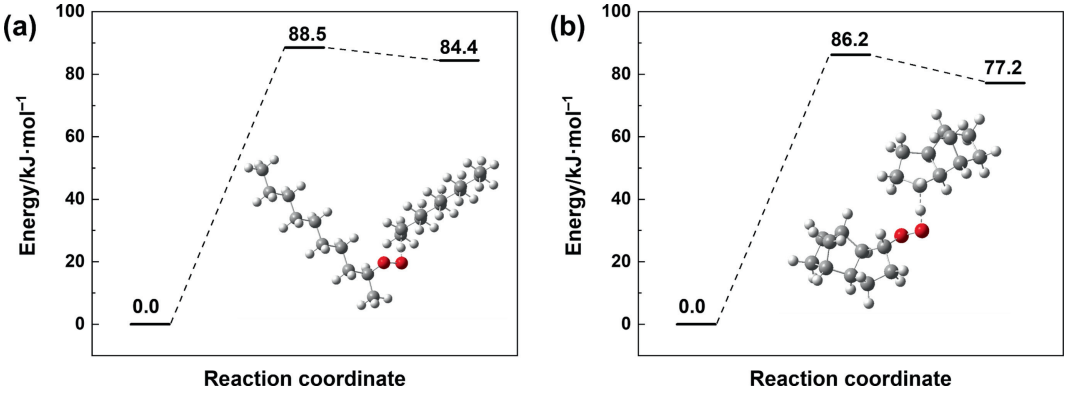

Fig. 2. Potential energy profiles of hydrogen abstraction for decane (a) and THDCPD (b) with the absence of diphenylamine. The inserts present the relevant TS structure.

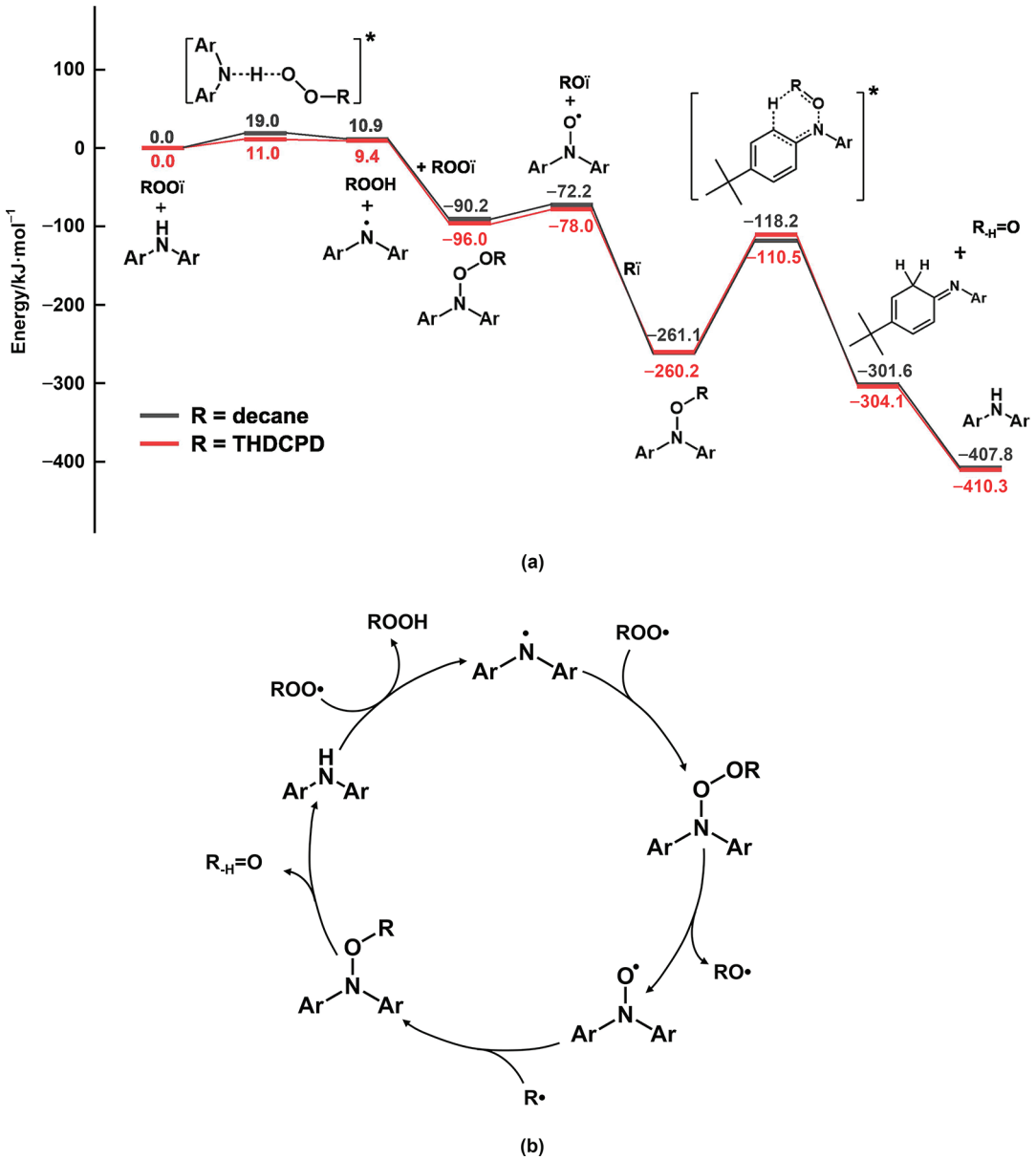

Fig. 3. (a) Proposed inhibition mechanism of diarylamine (Reproduced from Ref. [14], Copyright ©2014, American Chemical Society), (b) Calculated enthalpies for relevant structures in (a).

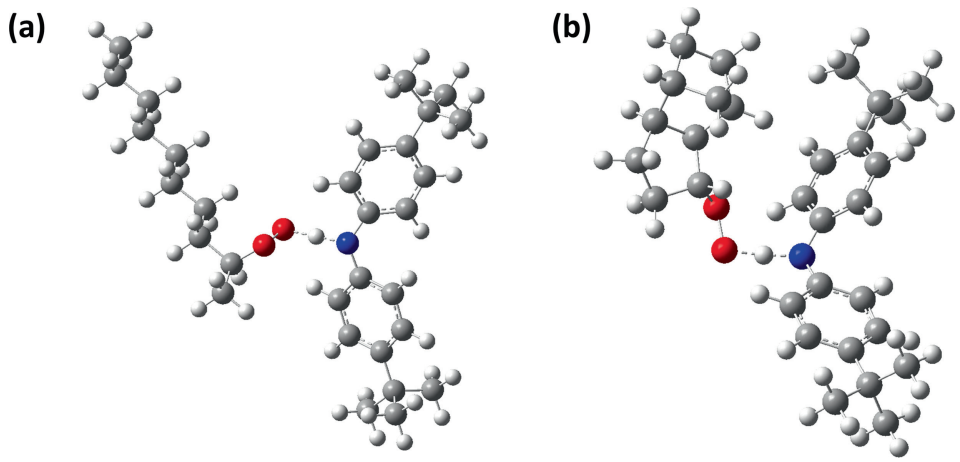

Fig. 4. Calculated TS structure for the reaction between diarylamine and peroxyl radicals of decane (a) and THDCPD (b).

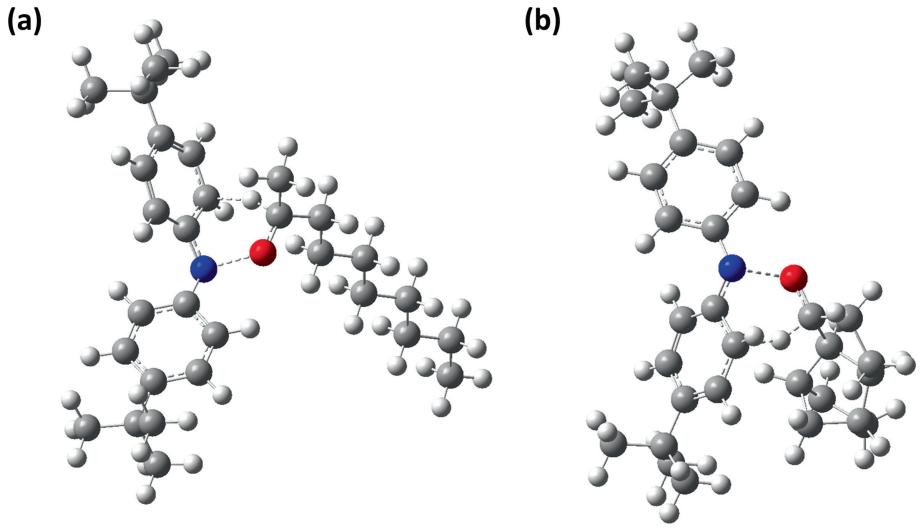

Fig. 5. Optimized TS structure for the retro-carbonyl-ene reaction during the oxidation of decane (a) and THDCPD (b) inhibited by diarylamine.

determining step in the regeneration of diarylamine. The high energy barrier of diarylamine regeneration corresponds to the unique efficacy of diphenylamine RTAs in high-temperature applications, *i.e.*, the high stoichiometric factor can only be achieved at elevated temperature. Importantly, the lower energy barrier of retro-carbonyl-ene reaction for diarylamine in decane suggests that diarylamine would be more efficient in preventing the oxidation of decane than THDCPD. Probably the multi-cyclic structure of THDCPD with relatively high steric hindrance hinders the retro-carbonyl-ene reaction.

3.2. Effect of diarylamine on fuel oxidation

To confirm the antioxidation activity of diarylamine, the experimental oxidation stability tests of decane and THDCPD with or without diarylamine addition were conducted by Rapid Oxy device. Fig. 6(a) and (b) respectively show the pressure curves inside the test chamber versus the time when different concentrations of diarylamine are added.

The results show that, for both pristine decane and THDCPD, the pressure drop occurs immediately after the pressure reaches a

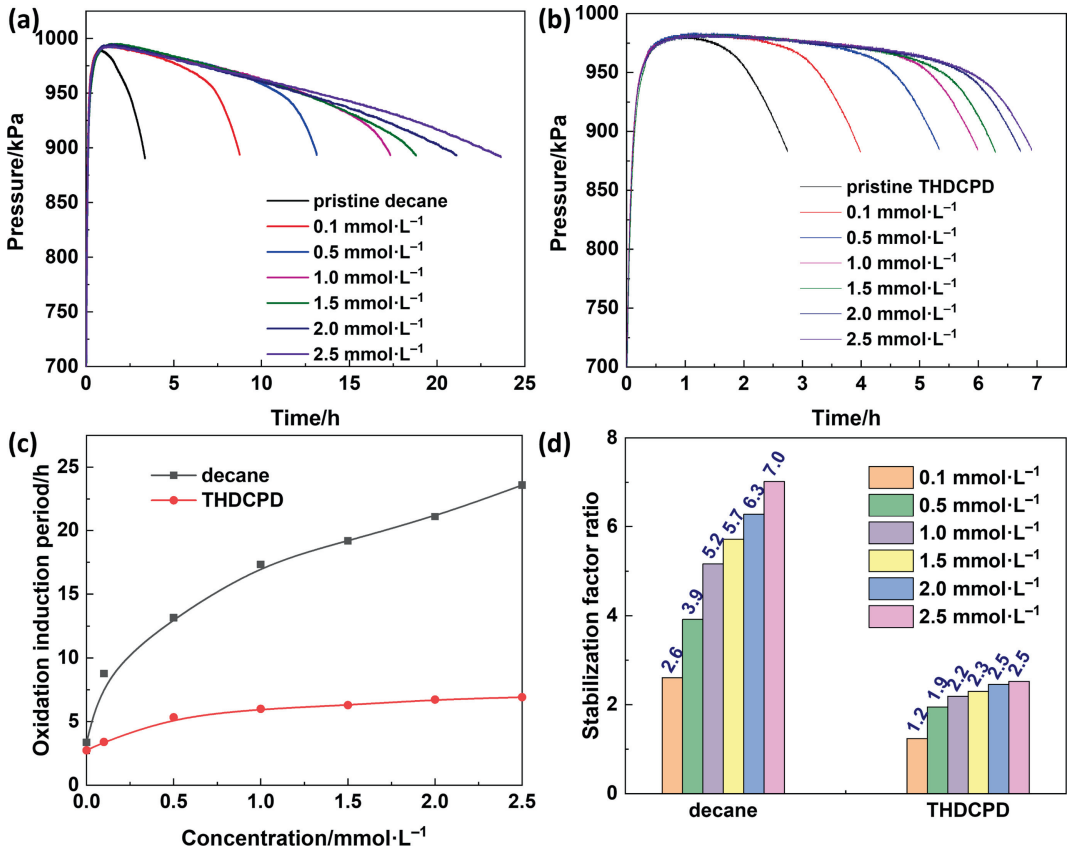

Fig. 6. Oxidation inhibition of decane and THDCPD by diarylamine. Oxygen pressure curves of decane (a) and THDCPD (b) with or without diarylamine in Rapid Oxy device versus time, (c) oxidation induction period versus diarylamine concentration and (d) stabilization factor ratio versus diarylamine concentration.

maximum value. As a result, pristine decane and THDCPD show analogous IP (Fig. 6(c)). With the addition of diarylamine, the pressure drops in the test chamber can be significantly inhibited, and accordingly, the IP of decane is prolonged from 3.4 h for pristine decane to 8.8 h for 0.1 mmol·L^{-1} and 13.2 h for 0.5 mmol·L^{-1} diarylamine addition. Importantly, the IP of decane can be further prolonged with the increase of diarylamine concentration, indicating that the addition of diarylamine can significantly increase the oxidation stability of decane.

The stabilization factor ratio (SFR) is introduced to express the antioxidant sensitivity, which is defined as the ratio of IP with antioxidant to IP without antioxidant (IP_0), *i.e.,* $SFR = IP/IP_0$ [43].

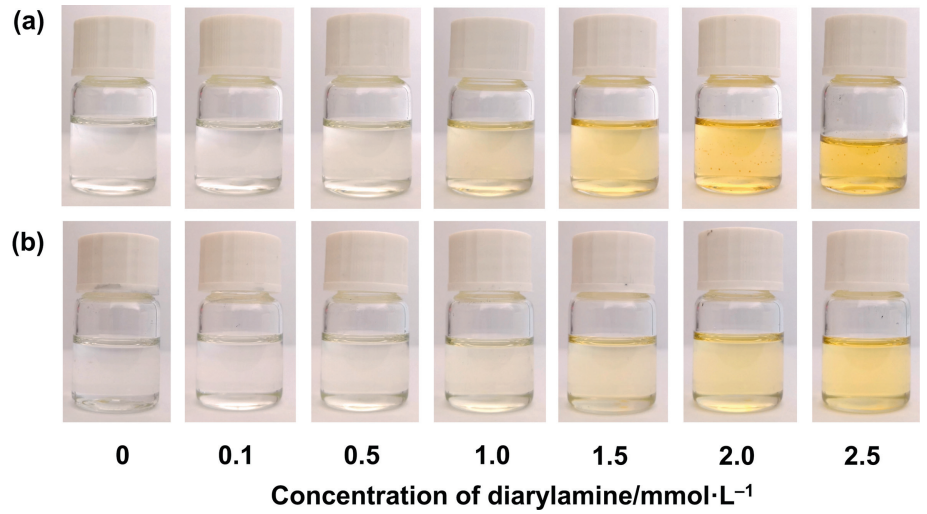

Fig. 7. Photographs of decane (a) and THDCPD (b) after accelerating oxidation with different concentrations of diarylamine.

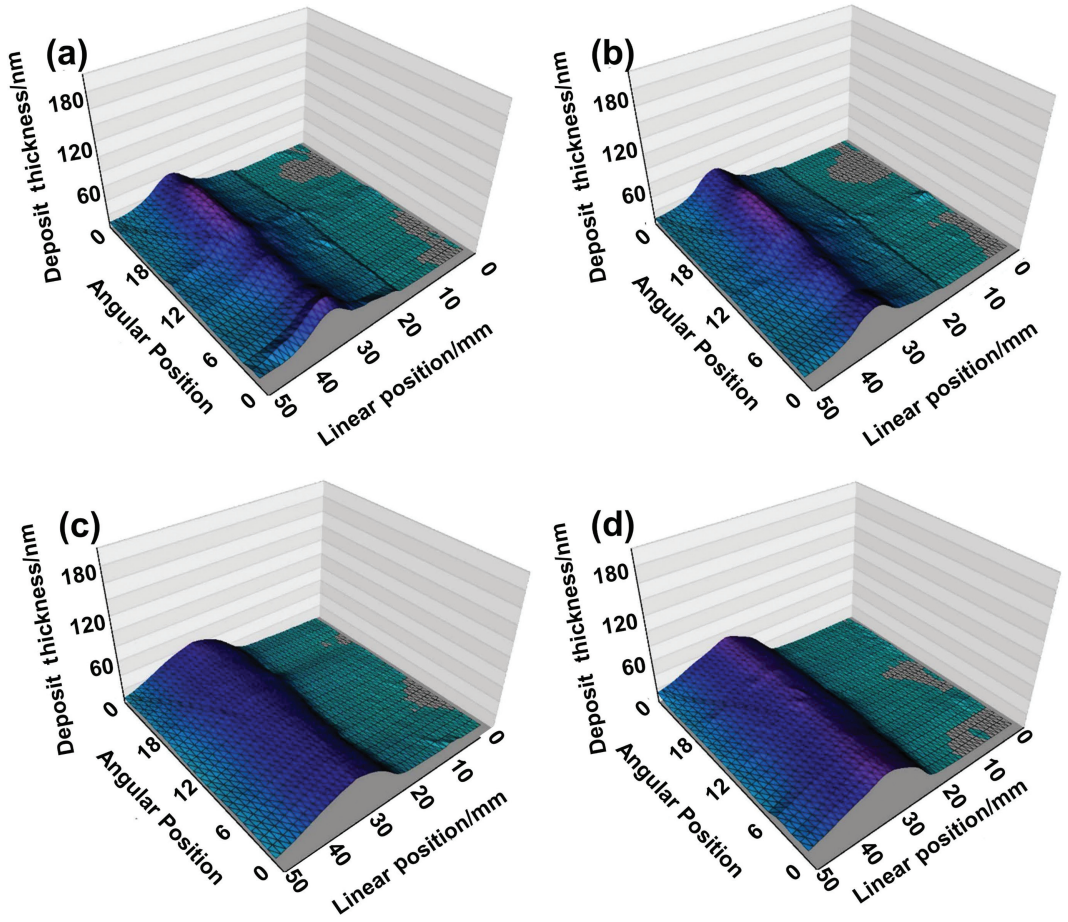

Fig. 8. Multi-angle film deposit profile of tubes after JFTOT test for (a) pristine decane, (b) decane with 0.5 mmol·L^{-1} diarylamine, (c) pristine THDCPD, and (d) THDCPD with 0.5 mmol·L^{-1} diarylamine.

From Fig. 6(d), the SFR of decane with 0.1 mmol·L^{-1} diarylamine addition is 2.6 and can be remarkably increased to 7.0 by adding 2.5 mmol·L^{-1} diarylamine. Although the addition of diarylamine can also mitigate the pressure drop of THDCPD, the IP is only extended from 2.7 h for pristine THDCPD to 3.4 h for 0.1 mmol·L^{-1} diarylamine addition. Moreover, the increase rate of IP for THDCPD is sharply weakened with the increase of diarylamine concentration, and as evidenced in Fig. 6(c), the IP is leveled off as the diarylamine reaches 1.0 mmol·L^{-1}. Accordingly, the SFR for THDCPD with 0.1 mmol·L^{-1} diarylamine addition is 1.2 and can only be increased to 2.5 with the addition of 2.5 mmol·L^{-1} diarylamine. These results are consistent with the preliminary calculation results that the addition of diarylamine can inhibit fuel oxidation and the diarylamine is more effective in inhibiting decane oxidation than that of THDCPD (Fig. 3(a)).

Fig. 7 shows the color change of decane and THDCPD with different concentrations of diarylamine after accelerating oxidation. Clearly, for both decane and THDCPD, the fuel samples with no diarylamine addition after accelerating oxidation exhibit no variation in appearance. However, the fuel samples (for both decane and THDCPD) with the addition of diarylamine turn into a light-yellow color but is still transparent after accelerating oxidation, and with the increase of diarylamine concentration, the color of the resultant fuel samples will be deepening. This result is different from our previous result that the addition of widely used BHT (2,6-di-*tert*-butyl-4-methyphenol, a hindered phenol) antioxidant will make almost no color deterioration [7]. Probably the formation of the side oxidative products of diarylamine, which can be chromophores, causes the obvious color change [44].

3.3. Effect of diarylamine on fuel deposition

The main problem of fuel oxidation is that it eventually leads to the formation of deposits, which will block fuel supply lines and ultimately cause catastrophic failure. According to the ASTM D3241, the jet fuel thermal oxidation tester (JFTOT) is the standardized method to rapidly assess the thermal oxidation stability (the resistance to the final deposition) of aviation fuels based on the pass/fail criterion (either the VTR exceeds 3 or the pressure drop across the stainless steel filter is higher than 25 mmHg corresponds to failure result), which subjects the test fuel to the flowing environment of high temperature and short residence time (approximately 5 s) that can simulate the practical condition. Therefore, the JFTOT was adopted for assessing the effect of diarylamine on jet fuel thermal oxidative deposition. For both decane and THDCPD with or without diarylamine, the tube ratings after JFTOT tests are assessed to be higher than 3 (not shown), indicating the failure results and inferior thermal oxidation stability. The ellipsometric tube rater (ETR) was further adopted to quantitatively evaluate the deposit thickness, and Fig. 8 shows the multi-angle film deposit profiles.

Fig. 9 summarizes the maximum thickness of deposits on the tested tube, the results show that the thermal deposition of pristine decane produces slightly more deposits than pristine THDCPD, indicating the more inferior thermal oxidation stability of decane than THDCPD, and importantly, for both two fuels, the addition of diarylamine can produce more severe deposition. From Fig. 9, with the addition of 0.5 mmol·L^{-1} diarylamine (approximately 140 mg·L^{-1}), the maximum deposit thickness of decane and THDCPD increases from 54.8 nm and 44.1 nm to 60.7 nm and 50.8 nm, respectively. This result indicates that diarylamine cannot mitigate fuel deposition but may cause slightly more deposits. According to our previous study [25], jet fuel thermal oxidative deposition propensity can be associated with the stability of oxidation intermediates, and the more stable the intermediates are, the fewer deposits will be produced. Normally, the added diarylamine

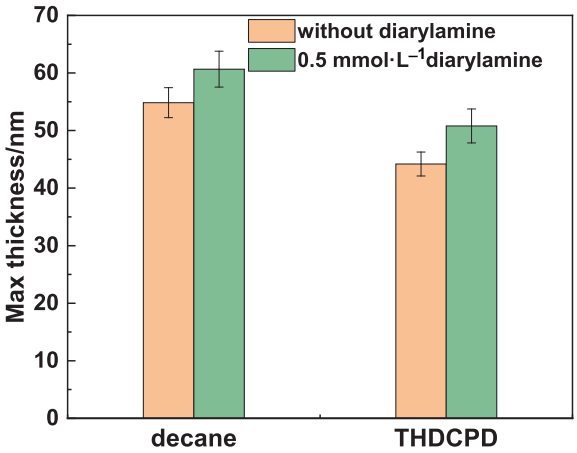

Fig. 9. The effect of diarylamine on the thermal deposition of decane and THDCPD.

can not only inhibit fuel oxidation but also can be regenerated during oxidation (Fig. 3(b) and 6), and thus the oxidation products of both jet fuel and diphenylamine can be avoided. However, the high-temperature thermal oxidative stress of diarylamine may inevitably produce several side products with high tendency to final deposits, such as *N*-phenyl iminoquinone [14]. In this case, dispersants should be urgently required to prevent the aggregation of deposit precursors and mitigate fuel deposition [8]. Even though, it is also worth noting that the flow condition, temperature regime, and surface characteristics in an aero-engine are substantially different in comparison with JFTOT, and thus the effect of diarylamine on jet fuel deposition should be carefully assessed for its validity in practical application.

4. Conclusions

In this work, the inhibition of two kinds of jet fuel (decane and THDCPD) oxidation by diarylamine was studied theoretically and experimentally. The diarylamine addition can significantly inhibit decane oxidation with the IP prolonging from 3.4 h to 13.2 h for 0.5 mmol·L^{-1} diarylamine addition but is less efficient for THDCPD. The DFT calculations reveal that the diarylamine will regenerate at elevated temperatures with the retro-carbonyl-ene reaction as the rate-determining step, and importantly, the energy barrier of retro-carbonyl-ene reaction in THDCPD is slightly higher than that in decane (142.9 kJ·mol^{-1} for decane *vs* 149.7 kJ·mol^{-1} for THDCPD), which causes the less efficiency of diarylamine in inhibiting THDCPD oxidation. In addition, the diarylamine will cause undesirable color change after accelerated oxidation and lead to slightly more deposits during high-temperature thermal oxidative stress for both decane and THDCPD. The results can provide significant implications for the future design of effective antioxidant additives to produce high-performance jet fuel.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors appreciate the financial support from the Postdoctoral Science Foundation of China (2021M702810), the Haihe Laboratory of Sustainable Chemical Transformations (CYZC202103),

and the National Natural Science Foundation of China (21978200 and 22222808).

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