ResearchGate

See discussions, stats, and author profiles for this publication at: https://www.researchgate.net/publication/251514137

Experimental study on the thermal decomposition of 2H-heptafluoropropane

ARTICLE *in* JOURNAL OF ANALYTICAL AND APPLIED PYROLYSIS · JANUARY 2011

Impact Factor: 3.56 · DOI: 10.1016/j.jaap.2010.10.006

CITATIONS
5

READS
53

5 AUTHORS, INCLUDING:

Tianfang Wang
University of the Sunshine Coast

52 PUBLICATIONS **200** CITATIONS

SEE PROFILE

Available from: Tianfang Wang
Retrieved on: 25 January 2016

Journal of Analytical and Applied Pyrolysis 90 (2011) 27–32

Contents lists available at ScienceDirect

Journal of Analytical and Applied Pyrolysis

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

Experimental study on the thermal decomposition of 2H-heptafluoropropane

Yonghua Hu[a,b,*], Yingbo Xu[a], Tianfang Wang[b,c], Chenghui Wang[a], Shufen Li[b,**]

[a] Technology Center, China Tobacco Anhui Industrial Corporation, Hefei, Anhui 230088, PR China
[b] Department of Chemical Physics, University of Science and Technology of China, Hefei, Anhui 230026, PR China
[c] Department of Chemistry, The University of Adelaide, Adelaide, South Australia 5005, Australia

ARTICLE INFO

Article history:
Received 9 October 2009
Accepted 18 October 2010
Available online 23 October 2010

Keywords:
2H-Heptafluoropropane
Thermal decomposition
FTIR
Acid–base titrate
Fluoride ion selective electrode

ABSTRACT

This is an extension study of the thermal decomposition of 2H-heptafluoropropane (HFP), mainly aiming at investigating the relationship between pyrolysis characteristics and reaction time, and evaluating the production of hydrogen fluoride (HF). The results indicate that reaction temperatures have obvious effects on the decomposition of HFP. Pure HFP does not decompose at 400, 500 and 600 °C. It starts to decompose at about 640 °C, markedly breaks down at 700 °C and exhibits intense decompositions at 800 °C; meanwhile, coke formation was observed on the inner surface of the reactor. Moreover, it can also be found that the reaction time has obvious effect on the thermal decomposition processes of HFP. From 700 to 800 °C the decomposition becomes increasingly drastic, and the concentration of HF produced highly depends on reaction temperature and time. This hints that when the total amount of HFP remains constant during practical application, the promotion of the spraying current capacity and the reduction of spraying time can reduce the production amount of HF, which can further lessen the harm to the personnel and the environment.

© 2010 Elsevier B.V. All rights reserved.

1. Introduction

Halon fire extinguishing agents, such as Halon-1301 (CF_3Br) and Halon-1211(CF_2ClBr), were widely used in the past due to their high flame inhibition efficiency. However, halons are potent ozone-depleting substances (ODSs) and synthetic green house gases (GHGs). The wide use of them has caused severe damage to the ozone layer and contributed significantly to the global warming [1–3]. In order to hasten the recovery of the ozone layer, international legislations, the Montreal Protocol and its Copenhagen Amendment, mandated the phase out of production and use of ODSs by all countries according to a specified timetable, which, in turn, has prompted a worldwide search for proper alternative fire suppressants that possess zero potential for ozone depletion yet are efficient in extinguishing a flame.

2H-Heptafluoropropane, commonly referred to as HFP or HFC-227ea, having the chemical formula of CF_3CHFCF_3, is believed to be a kind of ideal substitute, and used as fire-extinguishing agent more and more widely [4–6]. More than that, it can be used in a number of industrial applications, such as refrigerating medium, medical propellants, manufacturing of polymeric foams, and so forth. Under normal pressure, the property of pure HFP reveals itself to be a colorless and tasteless gas. The research has suggested that its global warming potential (GWP) is 0.3–0.5 and atmosphere lifetime (ALT) is 31–42 years, which are much better than those of halons. It is generally believed that the fire suppression mechanism of HFP is similar to that of halons, and can be separated to physical and chemical modes [4,7,8]. The physical contribution to flame suppression mainly stems from the heat-absorbing ability of the agent, which results in the flame temperature and the radical chain reaction rates decreasing in the flame. As to chemical suppression mechanism, some kinds of fluorine-containing free radicals would be formed during the thermal decomposition of HFP at the first stage; these radicals can react with the active radicals, e.g., O, H and OH, which play very important roles in the whole combustion process. This interrupts or terminates some key chain reactions that can be crucial for flame propagation. At the same time, some fluorocarbon compounds are generated, which have been proved to exhibit excellent fire suppression effects. Therefore, in order to understand its fire extinguishment mechanisms and properties, it is of significance to investigate the thermal degradation of HFP.

During the past decade, a series of experimental investigations have been carried out to study the thermal decomposition of HFP. Ritter [9] studied the pyrolysis of HFP mixture (2% HFP in nitrogen) at atmospheric pressure in the temperature ranging from 1023 to 1173 K, and 0–2 s reaction time in a quartz tubular flow reactor. It was found that HFP did not decompose appreciably at temperature below 1023 K and requires temperatures in excess of 1173 K for complete conversion, and major gas phase products included

* Corresponding author at: Technology Center, China Tobacco Anhui Industrial Corporation, 9 Tian Da Road, Gaoxin Zone, Hefei, Anhui 230088, PR China.
Tel.: +86 551 5738650; fax: +86 551 5392201.
** Corresponding author. Tel.: +86 551 3601137; fax: +86 551 3631760.
E-mail addresses: huyh@mail.ustc.edu.cn (Y. Hu), lsf@ustc.edu.cn (S. Li).

0165-2370/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.jaap.2010.10.006

perfluoropropene, pentaperfluoropropene, perfluorodimethylacetyene, hexafluoroethane, trifluoroethylene, tetrafluoroethylene and perfluoroisobutene. Moreover, solid products were also observed under their experimental conditions. Yamamoto et al. [10] investigated the pyrolysis of mixtures of 5% (V/V) HFP in air, and the decomposition products were analyzed using gas chromatography/mass spectrometry (GC/MS). The results showed that HFP began to decompose at 773 K, and it was nearly completely decomposed at temperatures of 973 K and disappeared at 1073 K. The main decomposition product was perfluoroisobutane. Hynes et al. [11] researched the kinetics of pyrolysis of HFP in dilute mixtures (0.5 and 3 mol% in argon) in a single-pulse shock tube within the temperature range of 1200–1500 K; residence times after the reflected shock and pressures were set to 650–850 μs and 16–18 atm, respectively. Reaction products were analyzed using GC/MS and FTIR techniques. They found that the most significant products detected were C_2F_6, $CF_2{=}CHF$, C_2F_4, C_3F_6, cyclo-C_3F_6, and CF_3CHCF_2H. Traces of CF_3H, CF_4, C_2F_5H, C_3F_8, C_4F_6, and isomers of C_4F_8 were also identified. Peterson and Francisco [4] theoretically studied the thermal decomposition pathways of HFP, and proposed a reaction model including twelve primary reaction pathways to describe the thermal decomposition mechanism of HFP.

We have previously studied the thermal decomposition processes of pure HFP at different temperatures (400, 500, 600, 700 and 800 °C) with the reaction time of 30 s, which showed that HFP would intensively decompose when the temperature reaches 700 °C, and the reaction basically terminates at 800 °C [12]. In addition, the effects of HFP on the flash pyrolysis products of PMMA, and the suppression ability of PMMA flame have also been preliminarily evaluated, and some interesting results have been proposed [13,14]. In order to comprehensively study the suppression mechanism of HFP and enhance its efficiency, the influence of spraying time (different reaction time) during a fire, which plays an important role, should be extensively studied. Also, the production of toxic substances should be worth paying more attention to. The aims of the present study are:

1. To use GC/MS, digital photograph and FTIR techniques to investigate whether variation of reaction time can affect the thermal decomposition of HFP. Such effects have not been studied experimentally or theoretically previously.
2. To use acid–base titrate and fluoride ion selective electrode methods to determine the concentration of HF formed during the thermal decomposition of HFP.

2. Experimental

2.1. Thermal decomposition procedures

HFP (99.9% pure) was supplied by Nanjing Fire Protection Technology Co. Ltd., and was not further purified before use. The thermal degradation runs were carried out in a furnace-type pyrolyzer. The experimental setup is shown in Fig. 1, and has been described elsewhere [12] in detail. In brief, for investigating the thermal decomposition of HFP in the present experimental condition, the pyrolytic degradation system mainly consists of a tubular heater with two exchangeable quartz tube reactors, a temperature programming control device and a suit of collecting assembly of products. The tubular heater can provide an about 10 cm length of uniform temperature profile (±5 °C). The temperature of the system is measured and controlled by the temperature programming control device with a K-type (chromel/alumel) thermocouple. Two different types of quartz tubes, whose internal diameters are 8 and 25 mm respectively, were used in order to obtain residence times of ca. 3 s and 30 s (with a 10 cm long uniform temperature zone and a flow rate of 100 ml/min). Before the experiment, the pyrolysis quartz tube was heated to 850 °C for 1 h to remove any contaminants. Then, the furnace was set to its desired temperatures ranging from 400 up to 800 °C. After the furnace had reached its set temperature, HFP gas was injected through the reactor at the rate of 100 ml/min. The products of the pyrolytic degradation were collected by a Cambridge pad assembly, a collection gas pocket and 50 ml of sodium hydroxide solution (0.723 mol/L) for 10 min, respectively.

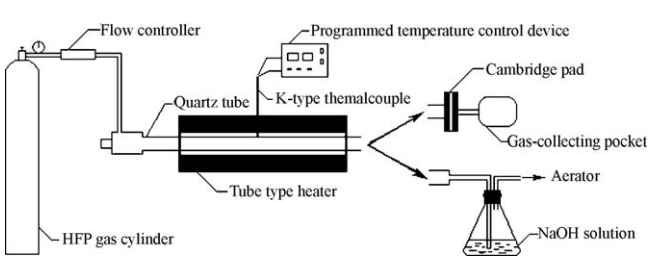

Fig. 1. The schematic of the experimental apparatus.

At the end of the thermal decomposition, the Cambridge pad was removed to a conical flask and extracted with 50 ml of dichloromethane (CH_2Cl_2) to dissolve the collected products. After being mechanically oscillated for 30 min, the CH_2Cl_2 extract was then filtrated. Before GC/MS analysis, the extract was transferred into a K.D. concentrator and concentrated to 1 ml at 60 °C.

2.2. FTIR analysis

Pure HFP and products collected by collection gas pocket were analyzed by FTIR spectrometer equipped with a deuterated triglycine sulfate (DTGS) detector and a 10-cm path length single-pass gas cell (MAGNA-IR750, Nicolet). The spectral range from 3500 cm^{-1} to 500 cm^{-1} was scanned, and 32 scans were co-added at 4 cm^{-1} resolution.

2.3. GC/MS analysis

Analysis of the products collected by the Cambridge pad was accomplished by a GC/MS (Agilent Techn., Inc., 6890GC/5973MSD) using HP-5MS capillary column(30 m × 0.25 mm i.d., 0.25 μm film thickness), with the following temperature programming: initial oven temperature was 30 °C; this was then raised to 150 °C at 4 °C/min, and held for 5 min. Helium was used as carrier gas with a flow rate of 1.5 ml/min (constant flow). Programming temperature vaporizer (PTV) injector temperature was 250 °C, and the amount of injection was 1.0 μl at spilt mode (spilt ratio, 20:1). The temperature of the GC/MS transfer line was 280 °C. The MSD was operated in the electron impact (EI) mode. The ion source temperature was 230 °C and the electron energy was 70 eV. The mass range from m/z 35 to 500 was scanned. The mass spectral identifications were carried out by comparing to the NIST02 mass spectral library as well as to the Wiley 275.L mass spectral library.

2.4. Acid–base titrate and fluoride ion selective electrode analyses

Hydrogen fluoride produced during the thermal decomposition of HFP was absorbed by 50 ml of sodium hydroxide solution (0.723 mol/L). The remaining sodium hydroxide was titrated with 0.701 mol/L of hydrochloric acid. According to the consumption of hydrochloric acid, the concentration of hydrogen ion in absorbent can be obtained.

The concentration of fluoride ion in absorbent was determined by using fluoride ion selective electrode method. Before the experiment, the fluoride standard solutions of 0.001, 0.005, 0.01, 0.05 and 0.1 mol/L were prepared by the serial dilution of a 0.1 mol/L sodium

fluoride solution. A calibration curve was created and corresponding equation is as follows:

$$E = -55.724 \quad \log[F^-] - 12.912 \quad r = 0.9999$$

where E is voltage value (mV), $[F^-]$ is the concentration of fluoride ion (mol/L), and r is the correlation coefficient.

The sodium hydroxide absorbent was directly analyzed by fluoride ion selective electrode, when the concentration of fluoride ion in the absorbent is low. In the case of the absorbent containing high concentration fluoride ion, it was diluted with deionized water before analysis. According to the voltage value and the above equation, the concentration of fluoride ion in absorbent can be calculated. Furthermore, the determination of the recovery rate of the fluoride standard sample was also performed in each analysis in order to verify the reliability of the analytical method. The results showed that all the recovery rates are in the range of 94.6–104.3%. Therefore, the good reliability of the method has been proved by experiment.

3. Results and discussion

3.1. FTIR spectrum of HFP

Fig. 2 (a) and (b) is FTIR spectra of pure HFP in the regions 3500–2000 cm^{-1} and 2000–500 cm^{-1}, respectively. Fig. 2 (a) reveals that there is a relative strong absorption peak at 2986.0 cm^{-1} assigned to the C–H bond stretching vibration [15]. In addition, numerous weak bands mostly belonging to overtones are also observed in Fig. 2 (a). The spectrum shown in Fig. 2 (b) illustrates that some strong bands, attributing mainly to C–F bond stretching vibration, exist over the wavenumber range 1400–1000 cm^{-1} [16]. In the case of two peaks at 908.3 and 859.4 cm^{-1}, their existence is contributed by C–H bond bending vibration [17]; while two absorptions at 741.9 and 689.7 cm^{-1} may be attributable to the skeleton vibration of three carbon atoms in HFP molecule. The spectra are consistent with those of McNaughton and Evans [15], which indicates that there are no impurities in HFP used in our research.

3.2. FTIR analysis results of products collected by collection gas pocket

With the residence time of 3 s, it is found that HFP does not decompose at 400, 500 and 600 °C, which has been confirmed by the fact that the FTIR spectra of the products collected in gas pocket and pure HFP are identical. In order to acquire the starting temperature of thermal decomposition of HFP, a series of pyrolytic experiments have been done in the temperature region of 600–700 °C. It has been found that when reaction temperature arrives at 640 °C with resident time of 3 s, a weak new absorption peak begins to appear at 3033.6 cm^{-1}, and its existence has been proven by two replicate experimental results, suggesting that the initial decomposition temperature for pure HFP is about 640 °C. Fig. 3 displays FTIR spectra of products collected by collection gas pocket during the thermal decomposition of HFP in residence time of 3 s, and at 640, 700 and 800 °C. It can be seen from Fig. 3 that the intensity of the new absorption peak has been obviously enhanced at 700 °C, in comparison with that of the peak at 640 °C. By increasing the temperature to 800 °C, there is many new peaks appear in spectrogram at 3053.4 cm^{-1}, 3013.4 cm^{-1}, 1794.4 cm^{-1}, 1751.0 cm^{-1}, 1328.5 cm^{-1}, 1152.4 cm^{-1}, 1034.9 cm^{-1}, 1029.8 cm^{-1} and 999.7 cm^{-1}. It is proposed that HFP has further decomposed and some products have formed at 800 °C.

Our previous results showed that pure HFP also does not decompose at 400, 500 and 600 °C with the residence time of 30 s [12], and the present results further demonstrate that pure HFP is also stable under such experimental conditions. Fig. 4 reveals that FTIR spectra of gas products in residence time of 30 s, and at 640, 700 and 800 °C. It can be found from Fig. 4 that at 640 °C, a relatively strong infrared absorption is observed at 3034.3 cm^{-1}, which demonstrates that HFP has obviously decomposed. At 700 °C, strong infrared absorptions are found at 3033.4 cm^{-1}, 1794.8 cm^{-1}, 1751.8 cm^{-1}, 1152.4 cm^{-1}, 1034.8 cm^{-1} and 1029.6 cm^{-1}, respectively, while relatively weak absorptions arise at 3053.3 cm^{-1}, 3012.9 cm^{-1}, 1336.4 cm^{-1} and 1003.0 cm^{-1}. The emergence of these new peaks indicates that HFP begins to intensively decompose at 700 °C, and some new fluorocarbon compounds are formed. At 800 °C, besides the above peaks, absorptions at 3115.0 cm^{-1} and 1195.8 cm^{-1} are newly identified, and there is also obvious variation for the overtone region. In addition, five strong peaks that assigned to the vibrations of C–H bond and three-carbons skeleton at 2986.0 cm^{-1}, 908.3 cm^{-1}, 859.4 cm^{-1}, 741.9 cm^{-1} and 689.7 cm^{-1} basically disappear, which can indicate that the pyrolysis of HFP is almost finished.

It has been generally accepted that the C=C stretching vibration of alkene can be detected within 1680–1620 cm^{-1} region, and the frequency will exhibit an obvious increment when one or more of the hydrogen on carbon substituted by fluorine, e.g., for $CH_2{=}CF_2$ and $CF_2{=}CF_2$, this absorption has been confirmed to increase to 1730 cm^{-1} and 1798 cm^{-1}, respectively [16]. In addition, Barnes et al. [18] have revealed that the $=CF_2$ group may possess the characteristic absorption at 1340 cm^{-1} and 1200 cm^{-1}. Accordingly, it can be recognized that emergences of 1794.8 cm^{-1}, 1751.8 cm^{-1},1336.4 cm^{-1} and 1195.8 cm^{-1} peaks at three experimental conditions, i.e., i) reaction time of 3 s at 800 °C, ii) reaction time of 30 s at 700 °C, and iii) reaction time of 30 s at 800 °C, are attributed to the formation of some fluoroalkenes. It should be mentioned that some fluoroalkene products may also undergo sub-degradations to form hydrogen fluoride and hydrogen-free fluoroalkenes in the three conditions.

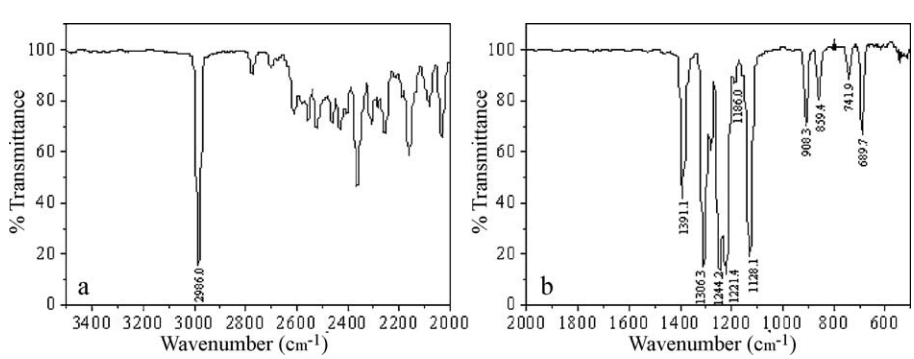

Fig. 2. FTIR spectrum of HFP.

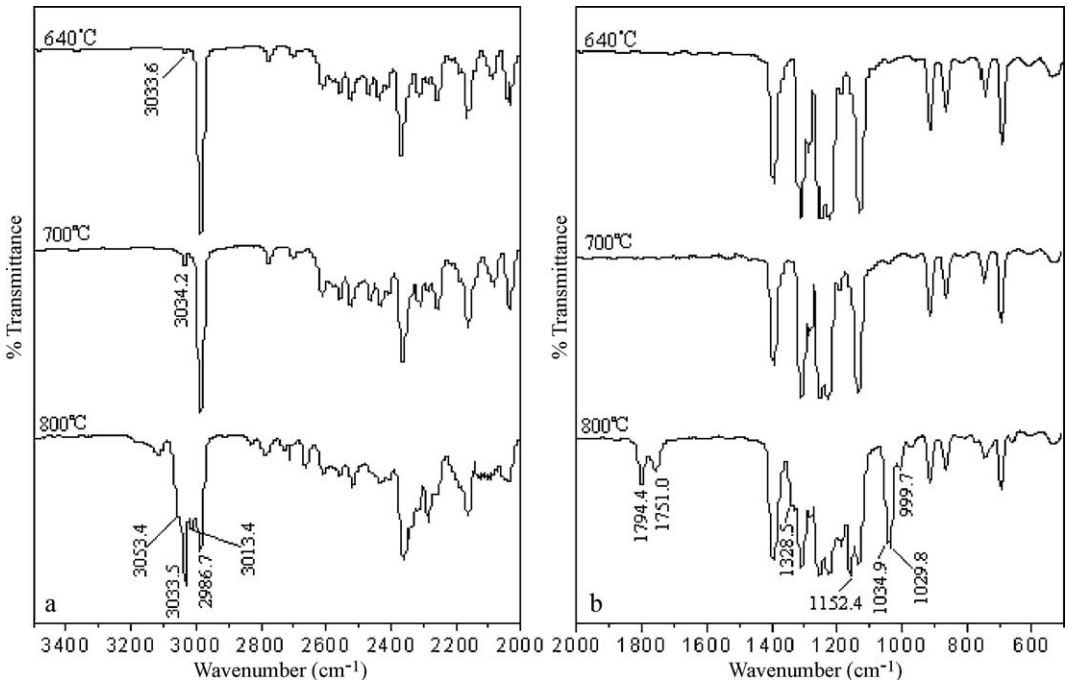

Fig. 3. FTIR spectra of products collected by collection gas pocket during the thermal decomposition of HFP in residence time of 3 s, and at 640 °C, 700 °C and 800 °C.

3.3. Products collected by the Cambridge pad and GC/MS analysis

The studies of the thermal decomposition kinetics of HFP carried out by Hynes et al. [11] have suggested that the pyrolysis products mainly include some small gas molecules, such as perfluoroethane (C_2F_6), 1,1,2-trifluoroethene (C_2HF_3), perfluoroethene (C_2F_4), hexafluoro-propene (C_3F_6), hexafluoro-cyclopropane (C_3F_6), 1,1,1,3,3,3-hexafluoro-propane ($C_3H_2F_6$) and so forth, and no compounds with relative large molecular weight have been detected. However, they have discovered that the carbon recovery percentage is decreased as the experimental temperature increases; based on this result, it has been proposed that there might be some more complex substances formed, or certain polymerization processes take place. While in our investigation, the Cambridge pad was used to capture this part of products. Fig. 5 shows the Cambridge pads at 800 °C with two residence times. There is no obvious color change for 3 s residence time (no color change can be observed for all the temperatures below 800 °C). However, it can be clearly seen that a great amount of flavescent oily liquids have been collected when the condition of 30 s reaction time at 800 °C was applied. This means that pyrolysis of HFP not only forms small gas molecules, but also involves the cyclization

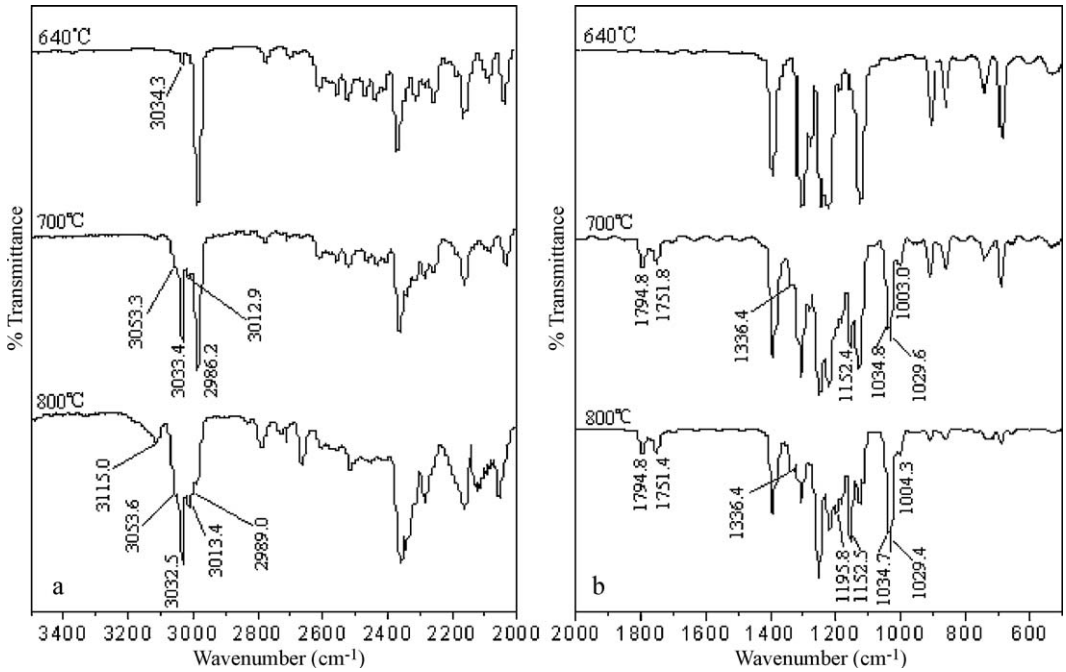

Fig. 4. FTIR spectra of products collected by collection gas pocket during the thermal decomposition of HFP in residence time of 30 s, and at 640 °C, 700 °C and 800 °C.

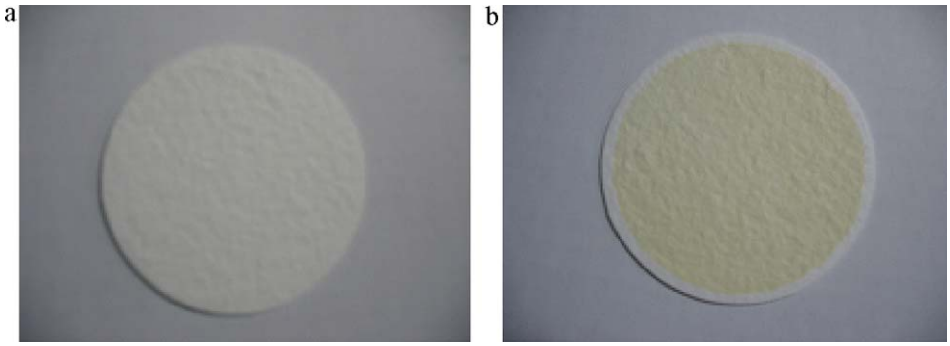

Fig. 5. The photos of products collected by Cambridge pad at 800 °C (a: residence time of 3 s; b: residence time of 30 s).

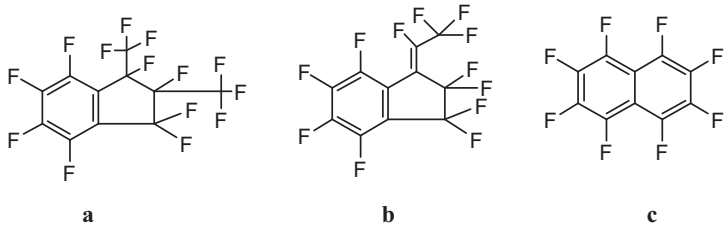

Fig. 6. Structures of three bicyclic compounds identified during the thermal decomposition of HFP [a: 1,2-bis(trifluoromethyl)perfluoroindane; b: perfluoro(1-ethylidene-indane); c: octafluoronaphthalene] [12].

and polymerization processes that can generate large molecules as well, which verifies the prediction of Hynes et al. directly.

Analysis of the products collected the Cambridge pad was accomplished by a GC/MS. The results suggest that there are basically no products which have been collected for the temperatures below 700 °C and residence time of 3 s at 800 °C. While abundant peaks arise in the case of 30 s and 800 °C, and three bicyclic compounds, such as 1,2-bis(trifluoromethyl)perfluoroindane, perfluoro(1-ethylidene-indane), octafluoronaphthalene, have been confirmed to exist [12], and their structures are shown in Fig. 6.

It has been widely acknowledged that small polycyclic compounds can act as the precursors of some large polycyclic compounds and coke [19]; thus, the structures displayed in Fig. 6 indicate the possibility of coke formation during the thermal decomposition of HFP. Though, due to the low concentration, these three molecules have not been identified out by GC/MS at 800 °C with resident time of 3 s, coke can already be seen on the inner-wall of quartz tube, which is in good agreement with the discovery of Ritter [9]. In addition to that, a great more coke is formed when the resident time increases to 30 s at the same temperature. The previous researches [20] have revealed that coke can cause the carbon-containing combustion products condensed, which accelerates the incarbonization of inflammable substances, and leads to insufficient combustion. Moreover, coke can also form a insulating condensed carbon layer on the combustion surface, and consequently restricts the heat and matter transfers between different phases. These two synergistic effects would favor the fire suppression. Therefore, it can be concluded that the formation of polycyclic compounds and coke in the thermal decomposition of HFP is favorable for promoting the fire-extinguishing ability.

3.4. Trends in the concentrations of hydrogen fluoride

There were also studies [21,22] focused on the toxicity of HFP, some of which have revealed that during the fire suppression processes utilizing HFP, a few noxious compounds would be formed, such as fluoride (F_2), hydrogen fluoride (HF) and carbonyl fluoride (CO_2F), etc. Amongst these substances, HF is usually generated with the highest concentration, and it can not only damage human's health, but also corrode facilities. Therefore, in order to reduce the formation of HF, its variation trends with different temperatures and resident times throughout the whole thermal decomposition processes of HFP should be of significant importance.

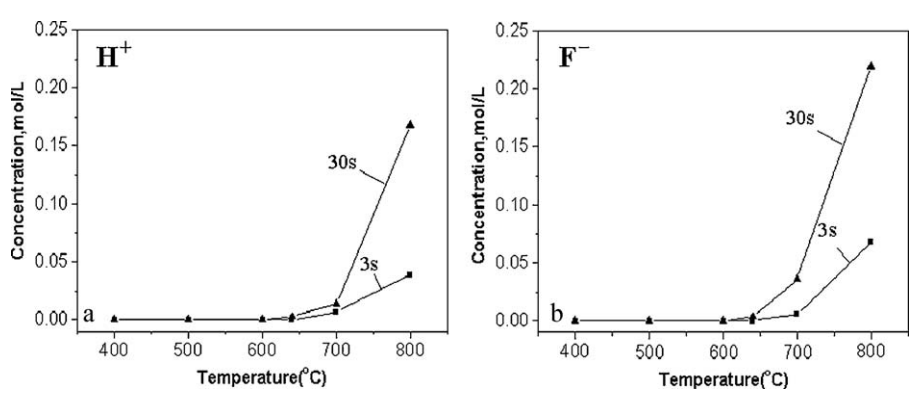

Fig. 7. [H^+] and [F^-] at different temperatures (400, 500, 600, 640, 700 and 800 °C) with resident times of 3 s and 30 s.

HF was absorbed in sodium hydroxide solution, and followed by acid–base titrate and fluoride ion selective electrode analyses to calculate [H^+] and [F^-], respectively. The results shown in Fig. 7 (a) and (b) suggest that the trends of [H^+] and [F^-] are quite similar though not being exactly the same. It can be found that [HF] nearly equals to zero below 600 °C, and [HF] exhibits a threshold when the temperature increases above 640 °C. With two resident times (3 s and 30 s), a sharp increment can be seen around 700 °C, and [F^-] reaches about 0.075 and 0.225 mol/L at 800 °C, respectively [see Fig. 7 (b)], which also indicates that resident time would affect the concentration of HF significantly. Consequently, given that the using certain amount of HFP during a fire suppression, it may be conjectured that decrease the spraying time can dramatically reduce the HF.

4. Conclusions

In this work, the thermal decomposition of pure HFP was investigated under the combinative conditions of 400–800 °C with reaction times of 3 s and 30 s. The products were analyzed by employing FTIR, GC/MS, acid–base titrate and fluoride ion selective electrode methods, respectively. Significant effects of the reaction temperature on the decomposition of HFP are confirmed to exist; pure HFP is stable below 600 °C, begins to decompose at about 640 °C and the decomposition would become obviously intense while the temperature keeps increasing up to 800 °C. In addition, the effects of the residence time on the thermal decomposition of HFP are also clearly observable. Accompanied by the temperature exceeding 700 °C, the concentration of the HF produced from the decomposition was found to evidently increase due to the enhancement of residence times. Therefore, when the total amount of HFP remains constant during practical application, the promotion of the spraying current capacity and reduction of spraying time can reduce the production amount of HF, which can further lessen the harm to the personnel and the environment. On the other hand, three cyclocompounds, i.e., 1,2-bis(trifluoromethyl)perfluoroindane, perfluoro(1-ethylideneindane) and octafluoronaphthalene, were discovered in products of the thermal decomposition at 800 °C and residence time of 30 s. Coke formation was observed on the surface of the reactor at 800 °C, which demonstrates that HFP not only takes place the simple decomposition, but also can undergo the cyclization and the polymerization reactions under high temperature thermal decomposition conditions. Furthermore, the formation of the cyclocompounds and coke can be in favor of suppressing a flame.

References

[1] K. Li, E.M. Kennedy, B.Z. Dlugogorski, Ind. Eng. Chem. Res. 38 (1999) 3345.
[2] H. Yu, E.M. Kennedy, M.A. Uddin, S.P. Sullivan, B.Z. Dlugogorski, Int. J. Chem. Kinet. 37 (2005) 134.
[3] R.F. Howe, S. Thomson, Y. Yang, K. Lee, E.M. Kennedy, B.Z. Dlugogorski, J. Mol. Catal. A: Chem. 181 (2002) 63.
[4] S.D. Peterson, J.S. Francisco, J. Phys. Chem. A 106 (2002) 3106.
[5] E.P.F. Lee, J.M. Dyke, W.K. Chow, F.T. Chau, D.K.W. Mok, Chem. Phys. Lett. 402 (2005) 32.
[6] J.Y. Liu, Z.S. Li, Z.W. Dai, X.R. Huang, C.C. Sun, Chem. Phys. 286 (2003) 173.
[7] M.L. Robin, Process Saf. Prog. 19 (2000) 107.
[8] M.L. Robin, Process Saf. Prog. 17 (1998) 209.
[9] E. Ritter, Chemical and Physical Processes in Combustion, Fall Technical Meeting, the Eastern States Section, 1997.
[10] T. Yamamoto, A. Yasuhara, F. Shiraishi, K. Kaya, T. Abe, Chemosphere 35 (1997) 643.
[11] R.G. Hynes, J.C. Mackie, A.R. Masri, J. Phys. Chem. A 103 (1999) 54.
[12] Y.H. Hu, S.F. Li, Spectrosc. Spectral Anal. 27 (2007) 2413.
[13] Y.H. Hu, S.F. Li, Fire Saf. Sci. 17 (2008) 34.
[14] T.F. Wang, Y.H. Hu, S.F. Li, D.L. Han, J. Anal. Appl. Pyrolysis 84 (2009) 39.
[15] D. McNaughton, C.J. Evans, Spectrochim. Acta, Part A 55 (1999) 1177.
[16] L.J. Bellamy, The Infrared Spectra of Complex Molecules, John Wiley, 1958.
[17] D.R.T. Appadoo, E.G. Robertson, D. McNaughton, J. Mol. Spectrosc. 217 (2003) 96.
[18] R.B. Barnes, R.C. Gore, R.W. Stafford, V.Z. Williams, Anal. Chem. 20 (1948) 402.
[19] H. Richter, J.B. Howard, Prog. Energy Combust. Sci. 26 (2000) 565.
[20] S.K. Durlak, P. Biswas, J. Shi, M.J. Bernhard, Environ. Sci. Technol. 32 (1998) 2301.
[21] J.Z. Su, A.K. Kim, M. Kanabus-Kaminska, Fire Saf. J. 31 (1998) 1.
[22] K. Omae, K. Oda, H. Nakashima, C. Ishizuka, H. Sakurai, K. Yamazaki, N. Saito, Y. Saso, Y. Ogawa, J. Occup. Health 40 (1998) 79.