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Performance Testing of Commercial Containers for Collection and Storage of Fire Debris Evidence

ABSTRACT: Fire debris evidence may contain ignitable liquid residues valuable in the investigation of a potential arson scene. The ability to obtain evidence containers that are contaminant-free and vapor-tight is essential to the analysis and storage of fire debris evidence. Commercial containers such as metal "paint" cans, glass mason jars, and polymer bags are often employed as fire debris evidence containers. The purpose of this research was to determine which of these three types of containers provided the most vapor-tight seal for the prevention of ignitable liquid vapor loss and to assess the potential for cross-contamination. Leak rates for each type of container were measured under controlled conditions. Simple mixtures of hydrocarbons were utilized in these experiments. Leak rates were determined based on the amounts of hydrocarbon recovered from activated charcoal located outside the test container and within a secondary container. Quantitation of the hydrocarbons recovered from activated charcoal was calculated using external standard calibration curves following analysis by gas chromatography–mass spectrometry. The results demonstrated that glass jars had the fastest leak rate followed by metal paint cans and properly heat-sealed polymer bags with the slowest leak rate. Each container exhibited a different leak mechanism, which resulted in an observable effect on the composition of hydrocarbons lost from the container. Hydrocarbon transfer from one container to another is also demonstrated. This study presents results that reveal the most vapor-tight container to be a properly heat-sealed copolymer bag.

KEYWORDS: forensic science, fire debris, evidence container

A commercial container must be contaminant-free and vapor-tight to be an effective fire debris evidence receptacle. The ignitable liquid residues found in fire debris consist mostly of volatile hydrocarbons. The demand for a vapor-tight evidence container is critical in retaining the ignitable liquid residues for further analysis. The containers recommended for fire debris evidence include metal "paint" cans with compression lids, glass mason jars with standard pressure-canning flats and bands, and special polymer sample bags (1–3). The advantages and disadvantages of each type of container are discussed in the second edition of *Practical Fire and Arson Investigation* (4). Various commercial containers for the collection and preservation of fire debris evidence have been investigated in the past (5–7). Most of the investigations examined the suitability of a specific container for fire debris storage by comparison with an accepted container. The most common hydrocarbon extraction method used in these investigations was the purge and trap onto charcoal, and the ignitable liquids chosen were relatively complex mixtures, including a petroleum distillate, gasoline, and a heavy petroleum distillate.

This study applies the hydrocarbon extraction method of passive headspace concentration of ignitable liquids onto activated charcoal as described in the ASTM E 1412 standard practice (8). Simple hydrocarbon mixtures of low molecular weight compounds were chosen for this study instead of the more complex ignitable liquids such as gasoline in order to facilitate the quantitation of leak rates and to simplify data interpretation. The main objective of this study was to determine which type of container (paint can, mason jar, or polymer bag) retains ignitable liquid vapors most efficiently.

This study utilized the method of passive headspace concentration of ignitable liquids onto activated charcoal, which can result in quantitative sampling errors unless care is taken to circumvent these problems. The effects of ignitable liquid volume, sampling time, sampling temperature, and activated charcoal size (surface area) on passive headspace concentration have previously been explored (9,10). The dynamic exchange of hydrocarbon molecules on the activated charcoal as well as any potential loss of the hydrocarbon molecules from the activated charcoal was examined as part of this study to reveal any effects these processes might have on the interpretation of the experimental results. Leak rates for metal "paint" cans, glass mason jars, and Kapak polymer bags were determined under carefully specified conditions. The influence of the rates and mechanism of leaking on the ratio of hydrocarbons recovered from an equimolar hydrocarbon mixture is demonstrated. In addition, the transfer of hydrocarbons from one closed container to another is also demonstrated, a result which could hold implications for sample cross-contamination.

Materials and Methods

A stock solution of hydrocarbons consisting of heptane, toluene, octane, nonane, and decane was prepared in an equimolar ratio of each hydrocarbon (i.e., the mole fraction of each hydrocarbon in the mixture was 0.20). A second, partially deuterated, stock solution of hydrocarbons consisting of heptane-d_{16}, toluene-d_8, octane, nonane, and decane-d_{22} was prepared in an equimolar ratio of each hydrocarbon. The toluene was purchased from Fisher Scientific (Pittsburgh, PA), the other hydrocarbons as well as *p*-xylene were purchased from Aldrich Chemical Co. (Milwaukee, WI). Low-benzene carbon disulfide was purchased from Fisher Scientific for desorbing hydrocarbons from the activated charcoal. Activated charcoal strips purchased from Albrayco (Cromwell,

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CT) were cut into 33.2 mm^2 area circular pieces using a hole-punch. The containers studied were quart metal paint cans, Ball® (Broomfield, CO) quart mason jars, and Kapak Fire DebrisPAK® (Minneapolis, MN) (cast nylon, acrylonitrile/methacrylate copolymer). The DebrisPAK® bags were cut to quart size volumes and large binder clips were inserted inside to prevent the bags from collapsing then heat sealed. Heat sealing was performed with the Kapak Corporation's pouch sealer, stock number 101-1, following the manufacturer's recommendations. The metal cans were sealed with compression lids and the mason jars fitted with standard pressure-canning flats and bands.

The first set of experiments, designed to investigate hydrocarbon exchange and loss from activated charcoal, utilized glass vial inserts super glued to the underside of a glass-evaporating dish providing support and stability to the vial insert. The vial inserts were used to contain the hydrocarbon mix and paperclip(s) holding activated charcoal disks. Three activated charcoal disks were perforated onto a paperclip which stood inside one of the empty vial inserts. The upside-down evaporating dish assembly was placed into a Ball® quart mason jar, as shown in Fig. 1*a*.

The second set of experiments, designed to investigate commercial container leak rates, placed a metal can, a mason jar, and a DebrisPAK® bag of quart volume (as described above) inside a full-sized DebrisPAK® bag. The full-sized bag also contained a paperclip with three activated charcoal disks suspended by dental floss from the heat seal, as shown in Fig. 1*b*.

The third set of experiments, designed to investigate the effect of a leaking container's closing mechanism on the hydrocarbon composition, placed a single container inside a full-sized DebrisPAK® bag along with three activated charcoal disks on a paperclip suspended by dental floss from the heat seal at the top of the bag, as shown in Fig. 1*c*.

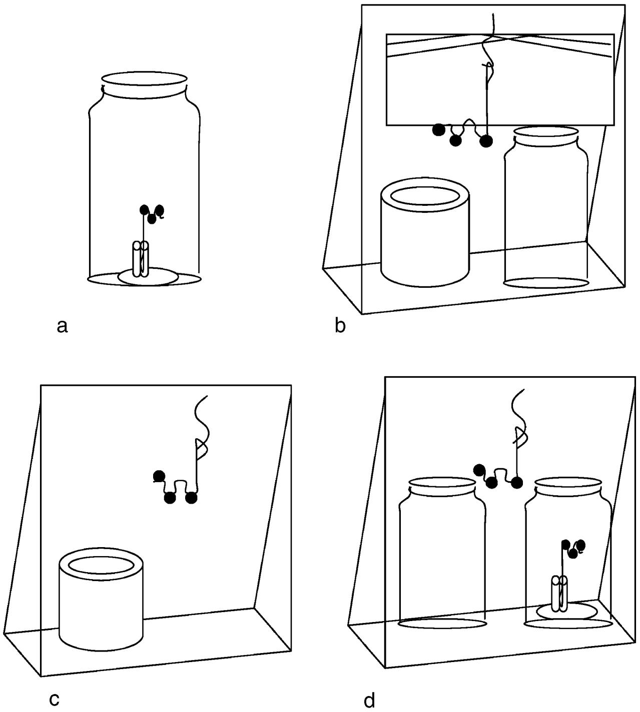

FIG. 1—*Diagrams showing the experimental setup including (a) Ball® glass mason jar with three activated charcoal disks; (b) a full-size Kapak Fire DebrisPAK® polymer bag containing a quart volume DebrisPAK® polymer bag, a quart volume metal paint can, a quart volume Ball® glass mason jar, and three activated charcoal disks; (c) a full-size Kapak Fire DebrisPAK® polymer bag containing a single quart volume container and three activated charcoal disks; and (d) a full-size Kapak Fire DebrisPAK® polymer bag containing two quart volume Ball® glass mason jars with multiple sets of three activated charcoal disks.*

The fourth set of experiments, designed to investigate cross-contamination of adjacent containers, placed two glass mason jars inside a full-sized DebrisPAK® bag with three activated charcoal disks inside one jar and three more activated charcoal disks on a paperclip suspended from the top of the bag, as shown in Fig. 1*d*.

The hydrocarbon sampling method used in these experiments was passive headspace concentration of ignitable liquids onto activated charcoal with desorption by carbon disulfide following the ASTM E 1412 standard practice. Equimolar hydrocarbon mixtures and pure hydrocarbons were deposited into vial inserts or test containers using a syringe or micropipet. Three activated charcoal disks were perforated onto a bent paperclip with clean-gloved hands. Containers were placed in a 66°C oven for various lengths of time then removed and allowed to cool to room temperature. The oven temperature chosen is within the temperature range suggested by the ASTM E 1412 standard. Furthermore, according to burn care professionals at Burnsurgery.org when outside temperatures reach 34°C (93°F), the temperatures inside a vehicle can reach 60°C within 40 min (11) and therefore the results presented here are representative of effects that can be observed upon prolonged holding of samples inside an automobile. The activated charcoal disks were removed from the paperclip with clean metal forceps and placed inside half-dram vials containing 1780 μL of carbon disulfide. Each activated charcoal disk extract was analyzed in triplicate. Control experiments demonstrated that 90–95% of the extractable hydrocarbons were eluted from the charcoal with a single CS_2 elution. In those control experiments a charcoal disk having adsorbed an equimolar hydrocarbon mix from the vapor phase at loadings below charcoal saturation, was sequentially eluted twice, following the protocols used for the experiments described here, and the first extraction was found to contain 90–95% of the total amount of extractable hydrocarbon. The protonated and deuterated hydrocarbons of each solution were identified by matching retention times and mass spectra with standards. An external standard method in which analyte mixtures of known concentrations are analyzed separately was utilized in creating calibration curves to quantify the hydrocarbons recovered from the activated charcoal. Control experiments in which empty, unused DebrisPAK® bags containing a charcoal strip were heated at 66°C for 16 h, demonstrated that the bags did not contribute any interfering compounds to the chromatograms. Control experiments in which an 8 cm^2 piece of DebrisPAK® bag were exposed to the equimolar hydrocarbon vapor at levels replicating the experiments described herein, with subsequent CS_2 extraction of the material, showed no retention of the hydrocarbons by the bag material.

The analyses were performed on an Agilent 6890 gas chromatograph with a 5973 mass-selective detector and a 7683 auto-sampler. Samples were chromatographed on a 25 m HP-1 methylsiloxane column with a 0.2 mm ID and 0.50 μm film thickness. Sample volumes of 1 μL were injected through a 250°C split/splitless injector with a 50:1 split ratio. The sample passed onto the chromatographic column at an initial temperature of 50°C, which was held for 3 min. The temperature was then increased at 10°C/min to a final temperature of 100°C and held for 2 min. The mass spectrometer was tuned according to the manufacturer's specification at a source temperature of 250°C. Spectra were scanned over a range of 30–350 *m/z* units.

Results

Hydrocarbon Molecule Exchange and Loss from Activated Charcoal

To investigate hydrocarbon molecule exchange on activated charcoal the following experiments were performed. Three paperclips with three charcoal disks each were placed inside a single jar, as shown in Fig. 1*a*, along with 10 μL of the protonated hydrocarbon mixture consisting of heptane, toluene, octane, nonane, and decane in equimolar ratio. After 22 h in the 66°C oven, one set of charcoal disks designated as set A was removed for analysis, whereas the other two sets, designated as B and C, were placed into clean unused jars (one set per jar). An additional 10 μL of the protonated hydrocarbon mixture was deposited in the jar containing charcoal disk set B, whereas 10 μL of the partially deuterated hydrocarbon mixture consisting of heptane-d_{16}, toluene-d_8, octane, nonane, and decane-d_{22} was deposited into the jar containing set C. The jars containing sets B and C were heated in the 66°C oven for 21 h then cooled to room temperature. Each set of charcoal disks were analyzed as described previously. This experiment was repeated with 18 μL volumes of the hydrocarbon mixtures and the activated charcoal disk sets designated as D (one exposure), E (second exposure with protonated mixture), and F (second exposure with deuterated mixture).

The average moles of adsorbed hydrocarbon eluted from each disk of set A (only one exposure to the hydrocarbon mixture) was 9.71×10^{-6} moles. The average moles of adsorbed hydrocarbon eluted from each disk of set C after exposure to the deuterated hydrocarbon mixture was 1.82×10^{-5} moles. The total hydrocarbon loading doubled upon second exposure to a hydrocarbon mixture, as shown in Fig. 2. Similar results were obtained from the set of B charcoal disks exposed twice to the protonated hydrocarbon mixture. The number of protonated heptane, toluene, and decane moles from set C charcoal disks remained the same between the first exposure to the protonated hydrocarbon mixture and the second exposure to their deuterated counterparts. It has previously been shown that 10 μL of hydrocarbon mix vapor will not saturate charcoal disks of this size (9). The experiment demonstrates additional adsorption of hydrocarbons at submonolayer coverage on the activated charcoal with no displacement or desorptive loss of the previously adsorbed hydrocarbons.

The experiment was repeated with 18 μL of the protonated and deuterated hydrocarbon mixtures. The average moles eluted from each disk of set D (only one exposure to the hydrocarbon mixture) was 1.87×10^{-5}. The average moles of adsorbed hydrocarbon eluted from each disk of set F, following the second exposure to the deuterated hydrocarbon mixture was 2.12×10^{-5}. Similar results were obtained from the set of E charcoal disks exposed twice to the protonated hydrocarbon mixture, but with further distortion of hydrocarbon profile. The eluted moles of protonated heptane, toluene, octane, and decane moles from set F charcoal disks decreased relative to the number of moles from set D, as shown in Fig. 3. It has been previously shown that volumes of hydrocarbon mixture greater than 18 μL will saturate charcoal disks of this size in quart volume containers (9). This experiment demonstrates desorptive loss and displacement of hydrocarbons once the activated charcoal is at or near the saturation limit.

In order to further demonstrate hydrocarbon loss from saturated charcoal the following experiment was performed. A paperclip with three charcoal disks was placed into a jar along with 10 μL of the protonated hydrocarbon mixture. A paperclip with three charcoal disks was placed in a second jar along with 18 μL of the protonated hydrocarbon mixture. Both jars were placed into a 66°C oven, then after 20 h one disk was removed from each jar for analysis. The paperclips with the remaining two disks were placed into clean unused empty jars and returned to the oven for an additional 20 h. The jars were then removed and the remaining charcoal disks were analyzed. A comparison of hydrocarbon moles from the disks exposed to 10 μL of hydrocarbon mixture revealed no loss of adsorbed hydrocarbons from the charcoal disks upon heating for the second period, as shown in Fig. 4. However, during the second heating period there was a loss of adsorbed hydrocarbons from the charcoal disks exposed to the 18 μL volume of hydrocarbon mixture, as shown in Fig. 5. The mole fractions of recovered hydrocarbons from all disks exposed to 10 μL of hydrocarbon mixture closely resembled the equimolar content of the liquid sample, as shown in Fig. 6. On the other hand, the mole fractions of recovered hydrocarbons from all of the disks exposed

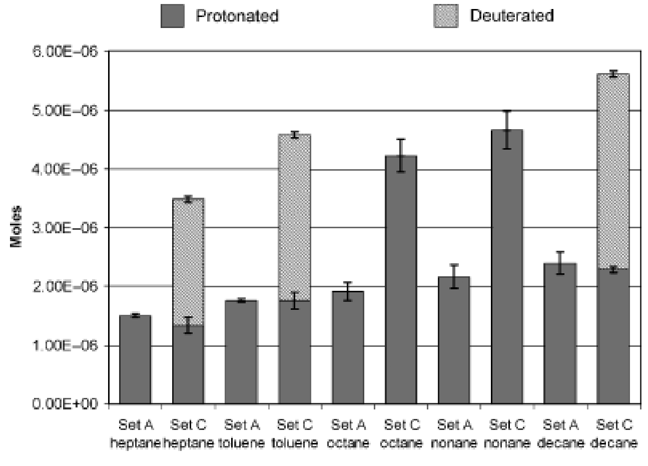

FIG. 2—*Moles of protonated adsorbed hydrocarbons eluted off charcoal disks from the first exposure to a 10 μL volume of protonated hydrocarbon mixture (Set A) and moles of protonated plus deuterated hydrocarbons eluted after additional 10 μL volume of deuterated hydrocarbon mixture (Set C). These results demonstrate additional adsorption of the hydrocarbons when the activated charcoal is below its saturation limit.*

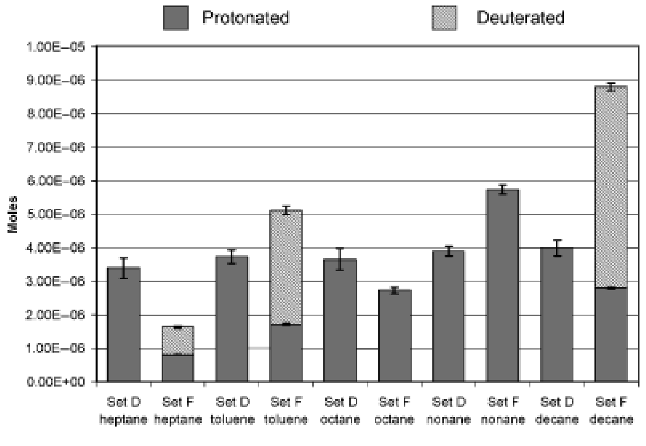

FIG. 3—*Moles of protonated adsorbed hydrocarbons eluted off charcoal disks from the first exposure to an 18 μL volume of protonated hydrocarbon mixture (Set D) and moles of protonated plus deuterated hydrocarbons eluted after additional 18 μL volume of deuterated hydrocarbon mixture (Set F). These results demonstrate displacement and loss of hydrocarbon molecules previously adsorbed onto the activated charcoal by the addition of more hydrocarbons once the activated charcoal has been saturated.*

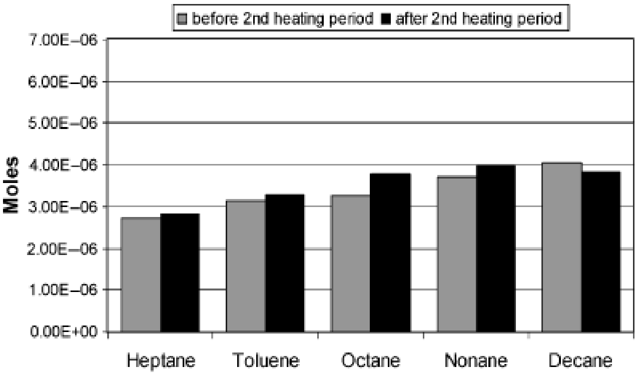

FIG. 4—*Moles of hydrocarbon eluted off charcoal exposed to a 10* µ*L volume of hydrocarbon mixture compared with hydrocarbon eluted from charcoal disks after a second heating period in a clean unused empty jar. These results demonstrate that the hydrocarbon molecules remain adsorbed onto activated charcoal after heating when the activated charcoal is below its saturation limit.*

to 18 µL of hydrocarbon mixture were not equimolar and indicated that displacement/loss had occurred. A significant change in the molar distribution was not observed after the second heating period even though a loss of each hydrocarbon occurred. This result also demonstrates that hydrocarbons adsorbed below the saturation level are *not* in equilibration with the headspace components on the timescale of the experiment.

Commercial Container Leak Rates

From the evaluation of nylon bags performed by the Centre of Forensic Sciences (12) and the recommendation from the manufacturer, the DebrisPAK® bags were heat sealed. Preliminary experiments indicated that the heat-sealed DebrisPAK® bag leaked less than the metal can and glass jar, so heat-sealed bags were utilized as the outer secondary container in the experiments, as shown in Fig. 1*b*. The concentration of each hydrocarbon in the headspace was calculated from the relationship between the vapor concentration and the amount of each adsorbed hydrocarbon that was eluted from the activated charcoal disks. An equal-volume hydrocarbon mixture consisting of toluene, toluene-d_8, and *p*-xylene, which have similar molecular weights, densities, and molecular structures was prepared. Volumes of 0.5, 4.5, 7.5, and 10.5 µL of the mixture were deposited into individual full-size DebrisPAK® bags each containing an empty quart-sized metal can, an empty glass quart jar, and an empty quart volume DebrisPAK® bag with three carbon disks suspended from the heat seal of the outer full-size bags. The four bags were all placed into a 66°C for 20 h, removed and the hydrocarbons desorbed from the charcoal disks with carbon disulfide. Under the experimental conditions, the entire volume of each deposited mixture was vaporized. After analysis, the ratio of each hydrocarbon (in ng) deposited into the outer DebrisPAK® bags was calculated relative to the amount of hydrocarbon (in ng) eluted from the charcoal disks. This ratio describes the relationship between the concentrations of each hydrocarbon in the headspace of the container to the hydrocarbons eluted from the charcoal disks, as shown in Fig. 7.

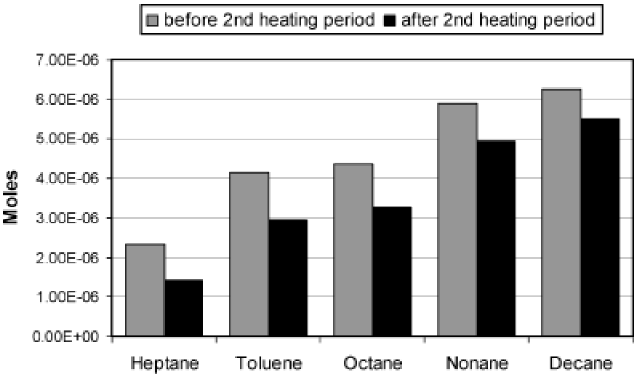

FIG. 5—*Moles of hydrocarbon eluted off charcoal exposed to a 18* µ*L volume of hydrocarbon mixture compared with hydrocarbon eluted from charcoal disks after a second heating period in a clean unused empty jar. These results demonstrate hydrocarbon molecule loss from the activated charcoal after heating when the activated charcoal is saturated.*

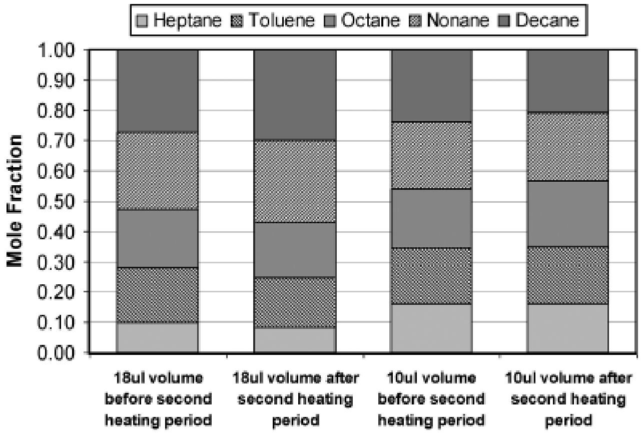

FIG. 6—*Mole fractions from adsorbed hydrocarbons eluted off charcoal disks before and after a second heating period in clean unused empty jars. These results demonstrate no significant change in the molar distribution of the hydrocarbons after the second heating.*

To determine container leak rates at 66°C, 5 µL of toluene-d_8, 5 µL of toluene, and 5 µL of *p*-xylene were individually deposited into a metal quart can, a glass quart jar, and a quart volume DebrisPAK® bag, respectively. Each assembly, as shown in Fig. 1*b*, included one of each type of container with its corresponding hydrocarbon along with three carbon disks in the outer secondary container. The assemblies were placed in the oven for 20, 50, 100, and 150 h with each assembly being duplicated at least three times. The amount of hydrocarbon leaking from each container was calculated based upon the calibration prepared for the

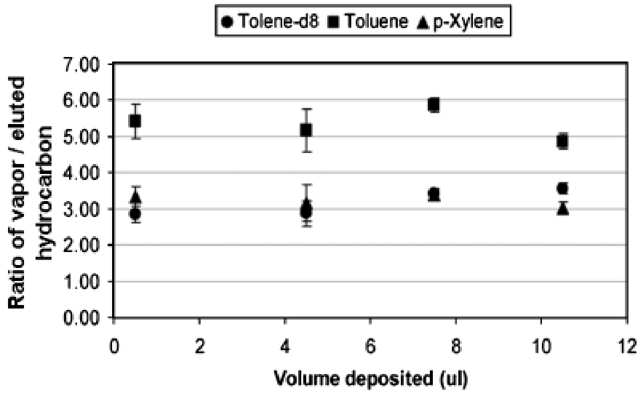

FIG. 7—*Ratio of each hydrocarbon deposited into the outer secondary DebrisPAK® bags, which vaporized to fill the headspace of the container, to each adsorbed hydrocarbon eluted off the charcoal disks. This ratio describes the relationship between the hydrocarbons in the headspace of the container to the adsorbed hydrocarbons recovered by elution off the charcoal disks.*

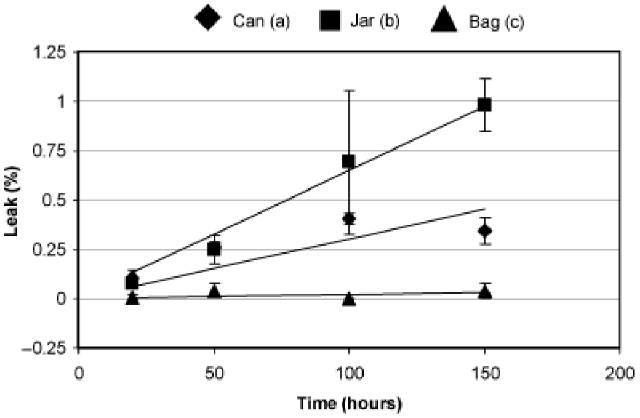

FIG. 8—*(a) Leak rate for metal paint cans, 3.0 × 10^{-3} mol%/h, (b) leak rate for Ball® glass mason jars, 6.5 × 10^{-3} mol%/h, and (c) leak rate for DebrisPAK® polymer bags, 2.0 × 10^{-4} mol%/h.*

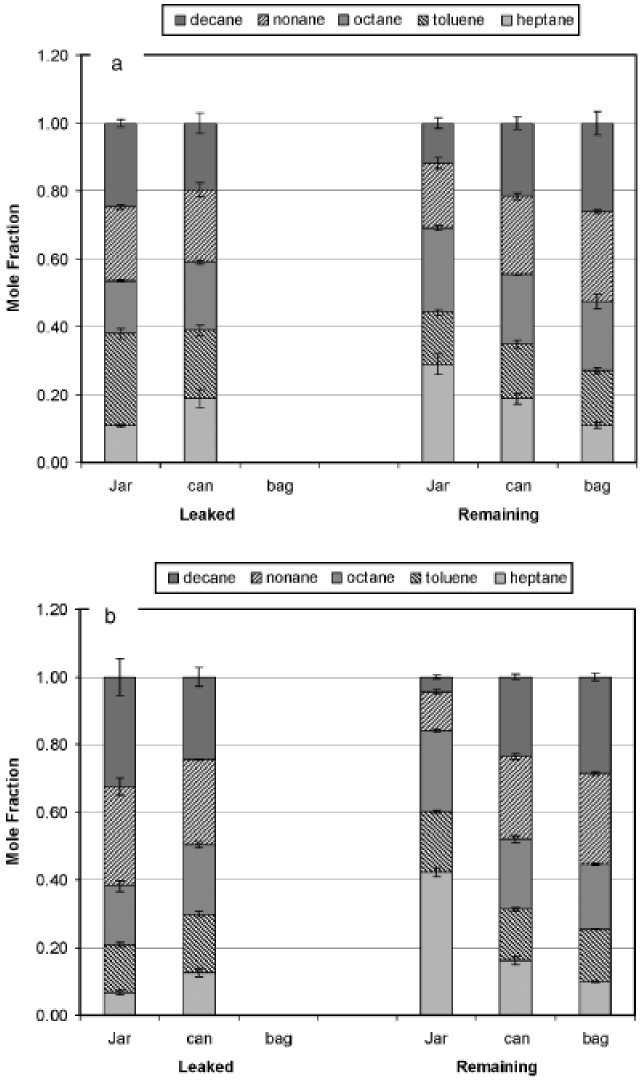

FIG. 9—*Hydrocarbon mole fractions which leaked from the containers and those that remained inside of the container, (a) 10 μL volume, (b) 18 μL volume. These results demonstrate the effect each container leak mechanism has on the composition of an equimolar hydrocarbon mixture.*

experiment, as described in the previous paragraph. The percent leak for each container was determined to be an approximate linear function of time, i.e., zero-order kinetic behavior. The leak rates for the metal cans, glass jars, and DebrisPAK® bags were found to be 3.0 × 10^{-3}, 6.5 × 10^{-3}, and 2.0 × 10^{-4} mol%/h, respectively, as shown in Fig. 8. The glass mason jars demonstrated the fastest leak rate followed by the metal paint cans and the slowest leak rate was observed for the DebrisPAK® bags. The DebrisPAK® bags did not leak significantly when properly heat sealed, but when the bag was not sealed correctly the leak rate increased substantially. One bag of 12 used in these experiments failed to seal properly, providing clearly anomalous results. It was determined that the leak rates did not change significantly when the hydrocarbons were redistributed among the different container types (i.e., toluene-d$_8$ in jar, toluene in DebrisPAK® bag, and *p*-xylene in can).

In order to determine if a container leak has an effect on the composition of a hydrocarbon mixture, a 10 μL volume of an equimolar hydrocarbon mixture containing heptane, toluene, octane, nonane, and decane was deposited into a jar, can, and bag of quart size volume and sealed appropriately. Each of these containers was placed inside an individual full-sized DebrisPAK® bag containing three activated charcoal disks suspended from the top of the bag by a paperclip and dental floss, as shown in Fig. 1*c*. Each of the three container assemblies was duplicated with an 18 μL volume of the same equimolar hydrocarbon mixture. The bags were placed in a 66°C oven for 146 h, then removed and allowed to cool to room temperature. The charcoal disks were analyzed to determine the mole fractions of each hydrocarbon which leaked from each of the containers. Then, each container was placed inside a new individual DebrisPAK® bag containing a new set of three charcoal disks. Immediately before heat sealing the outer bag, each of the containers was opened allowing the hydrocarbon molecules retained inside each container to be adsorbed onto the new activated charcoal. The bags were placed inside a 66°C oven for 20 h, then removed and allowed to cool to room temperature. The charcoal disks were analyzed to determine the mole fractions of the hydrocarbons which had not leaked from the containers during the first 146 h heating period. The DebrisPAK® bag containers were found not to leak, whereas the glass jar and metal paint can did leak as demonstrated by the hydrocarbon mole fractions extracted from the activated charcoal disks, as shown in Fig. 9.

Possible Cross-Contamination of Containers

Two experiments designed to test for hydrocarbons passing from one closed container into another closed container (cross-contamination) were conducted with glass mason jars. In the first experiment, a full-size DebrisPAK® bag was prepared containing two glass mason jars, a set of three activated charcoal disks suspended from the heat seal, and 10 μL of toluene-d$_8$. One jar contained three activated charcoal disks on a paperclip with no hydrocarbon liquid and the other jar contained 50 μL of toluene deposited into a vial insert, as shown in Fig. 1*d*. The whole assembly was placed in a 66°C oven for 163 h then allowed to cool to room temperature. After the activated charcoal disks were analyzed, it was determined that toluene constituted 70% of the hydrocarbons recovered from the outer DebrisPAK® bag and the jar that originally contained no hydrocarbon liquid had an equal quantity of both toluene and toluene-d$_8$, as shown in Fig. 10.

The second experiment utilized the same two jars inside a bag assembly as described in the previous paragraph, except that in this experiment 50 μL of toluene was deposited into one jar and 50 μL of toluene-d$_8$ was deposited into the second jar with no

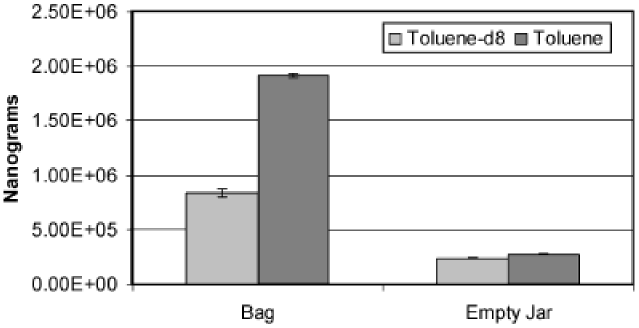

FIG. 10—*Amounts of toluene leaked from a Ball® glass mason jar into the outer bag and transfer to an empty Ball® glass mason jar. Toluene-*d_8 *deposited into the outer bag was detected inside the empty Ball® glass mason jar. These results demonstrate the ability of hydrocarbons from a leaking Ball® glass mason jar or the environment can penetrate an empty Ball® glass mason jar.*

toluene or toluene-d_8 placed in the outer bag. Each jar and the outer bag contained a set of three activated charcoal disks. The assembly was placed in a 66°C oven for 192 h then allowed to cool to room temperature. After analysis, both toluene and toluene-d_8 were recovered from all of the activated charcoal disks. The major constituent in each jar was the hydrocarbon which was originally deposited inside the jar as a liquid, as shown in Fig. 11.

Discussion

Hydrocarbon Molecule Exchange and Loss from Activated Charcoal

These experiments were performed to gather a better understanding of the adsorptive and desorptive processes of the hydrocarbon molecules and the activated charcoal. The results provided a means of developing a suitable method and proper interpretation of the results for the container leak rate experiments. At low volumes (i.e., 10 μL) of hydrocarbon mix, the activated charcoal disks are not saturated with hydrocarbon. Under these conditions, the adsorbed hydrocarbon molecules are retained on the activated charcoal, even when the activated charcoal is reheated inside a clean container. Additional hydrocarbon molecules are adsorbed onto the charcoal disk after another 10 μL of hydrocarbon mix is deposited into the container, leading to saturation of the adsorption sites and resulting in distortion of the hydrocarbon profile (9), as shown in Fig. 2. At higher initial spiking volumes (i.e., 18 μL of hydrocarbon mix), the activated charcoal disks are saturated resulting in a distorted hydrocarbon profile (i.e., the hydrocarbons are no longer equimolar). A second 18 μL spike results in further distortion, as shown in Fig. 3. These results are explained by the hydrocarbon molecules first filling the adsorption sites of the activated charcoal to form a "monolayer." Subsequent, displacement occurs leading to loss of the less strongly adsorbed hydrocarbons. Adsorption occurs primarily through dispersion interactions between the hydrocarbons and the activated charcoal (8).

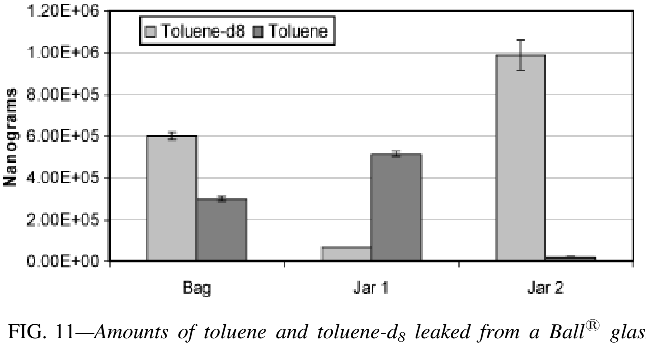

FIG. 11—*Amounts of toluene and toluene-*d_8 *leaked from a Ball® glass mason jars into an outer bag and the cross-contamination between the two jars. The results demonstrate that it is possible for hydrocarbons from two adjacent Ball® glass mason jars to leak and penetrate the other jar.*

Commercial Container Leak Rates

At 66°C the glass mason jar leaked at the fastest rate followed by the metal paint can, then the DebrisPAK® bag showing the slowest leak rate. Within the first 50 h the leak rates of the glass mason jars and metal paint cans were indistinguishable; however, subsequent monitoring showed the mason jars leak at a faster rate than the metal paint cans. After 6 days at 66°C, 98% of the hydrocarbon in the mason jar had leaked from the container. The DebrisPAK® bags with the heat seal did not leak significantly, with the exception of a single bag that was found to have been improperly sealed.

An examination of an equimolar hydrocarbon mixture over a period of several days demonstrated different leaking mechanisms for each type of container. Typically a 10 μL volume of hydrocarbon mixture does not saturate an activated charcoal disk in a quart volume container at 66°C for a 20-h period. The first set of activated charcoal disks collected the hydrocarbons which leaked from the container. The second set of activated charcoal disks measured the hydrocarbons which remained inside the container. The mole fractions from each set of activated charcoal disks were calculated to reveal the relative hydrocarbon composition. The hydrocarbons within the glass jar did not escape at equal rates. The hydrocarbon with the smallest collision diameter leaked at the fastest rate, whereas those with larger collision diameters leaked at slower rates. According to the USDA Complete Guide to Home Canning, "the lid gasket softens and flows slightly when heated to cover the jar-sealing surface, yet allows air to escape from the jar" (13). The hydrocarbons within the metal can leaked equally thus, leaving equimolar amounts remaining within the can. The DebrisPAK® bag did not leak, so all of the hydrocarbons of the equimolar mix remained inside the bag; however, the mole fractions of the recovered hydrocarbons were not equal as expected, perhaps a result of the extended period of heating. An 18 μL volume of hydrocarbon mixture in a quart volume container at 66°C for a 20-h period may saturate the activated charcoal disk resulting in a distortion effect on the hydrocarbon profile. The distortion effect appears to have been reduced for the metal paint can possibly due to similar leak rates for each hydrocarbon. The leak rates for the hydrocarbons in the metal can reduced the total amount of the hydrocarbons remaining in the container, thereby preventing saturation of the activated charcoal disk and avoiding displacement which leads to a distortion of the hydrocarbon profile.

Possible Cross-Contamination of Containers

Over several days at 66°C, a glass mason jar will leak allowing hydrocarbons to escape from the container and subsequently enter into an empty jar. Hydrocarbons from the surrounding environment may also enter into the empty jar. The performance of the glass mason jar lids may vary from container to container, as shown in Fig. 11.

In this study, the properly heat-sealed copolymer bags retained all of the hydrocarbons. However, it is unknown whether other liquids such as oxygenates behave in a similar manner. The other two containers leaked losing the hydrocarbons in different proportions due to their individual closing mechanisms thus changing the hydrocarbon composition and chromatographic profile. Over time, leaking jars containing hydrocarbons can cross-contaminate one another if stored in close proximity and hydrocarbons from the immediate environment can penetrate the jar.

Acknowledgments

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