EXPERIMENTAL AND NUMERICAL EVALUATION OF ELECTROTHERMAL–SWING ADSORPTION FOR CAPTURE AND RECOVERY OR DESTRUCTION OF ORGANIC VAPORS

BY
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DISSERTATION
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ABSTRACT

Emissions of hazardous air pollutants (HAPs) and volatile organic compounds (VOCs) to the atmosphere are serious environmental issues. There were 5.3x10^8 kg of HAPs and 1.5x10^{10} kg of VOCs emitted to the atmosphere from anthropogenic sources during 2004 and 2002, respectively (USEPA, 2007a, 2007b). Eighty-nine percent of those HAPs were emitted from point sources that can be readily captured by techniques such as adsorption (USEPA, 2007a). The cost to meet regulations for VOC control during 2010 was estimated at $2.3 billion/yr (USEPA, 1999). Environmental regulations encourage the development of new technologies to more effectively remove HAPs/VOCs from gas streams at lower cost. Electrothermal Swing Adsorption (ESA), as described here, is a desirable means to control these emissions as it allows for capture, recovery and reuse or disposal of these materials while providing for a more sustainable form of technological development.

The Vapor Phase Removal and Recovery System (VaPRRS or ESA-R)) was initially evaluated for possible improvements. An automated bench-scale adsorption device using activated carbon fiber cloth (ACFC) was designed and built to study effects of select independent engineering parameters on the ability of the system to capture and recover an organic vapor (e.g., methyl ethyl ketone, MEK) from air streams. Factors that can increase the adsorbate liquid recovery with low energy costs were investigated using sequentially designed sets of laboratory experiments. Initially, the screening experiments were conducted to determine significant factors influencing the energy efficiency of the desorption process. It was determined that “concentration of organic vapor”, “packing density”, and “maximum heating temperature” are significant factors while “nitrogen flow” and “heating algorithm” are insignificant factors in the ranges of values that were evaluated. Experimental data provided from this work were then used as inputs by Kaldate (2005) to complete a response surface methodology using Central Composite Design to optimize the operation of the ESA system in a region where efficient liquid recovery can be achieved. These results were used by Kaldate (2005) to reduce the amount of power applied per unit mass of ACFC in the vessel and provide a scale-up
model of the ESA system.

A comparison between experimental bench-scale VaPRRS and a pilot-scale VaPRRS was also completed as part of this research. Results from this effort demonstrated that both the bench-scale and pilot-scale ESA systems had removal efficiencies of MEK > 98%. The average electrical energy per unit mass of recovered liquid MEK was 4.6 kJ/g and 18.3 kJ/g for the bench unit and pilot unit, respectively.

A new concentration controlled desorption device, known as ESA-Steady State Tracking (ESA-SS) desorption, was also designed and built as a bench-scale laboratory device as part of this research. This new system was demonstrated to operate over a wide range of conditions (i.e., type of organic vapor, concentration of organic vapor, ratio of desorption/adsorption cycle gas flow rates, fixed and dynamic desorption concentration set-points, constant and variable inlet concentration of organic vapor, batch and cyclic modes, and with dry and humid gas streams). It was shown that concentration of organic vapor that is generated during regeneration cycles can readily be controlled at concentration set-points for three organic compounds (MEK, acetone, and toluene). The average absolute errors (AAEs) were < 5% when comparing the set-point and the measured outlet vapor concentrations. This is the first time that such performance has been demonstrated and this performance is not possible with other current technologies. Such capability of the system allows a secondary control device to be optimized for select constant concentrations and much lower gas flow rates (e.g., 5% of the gas flow rate during the adsorption cycle) that is not possible without such pretreatment.

An ESA-Concomitant Adsorption and Desorption (CAD) system was also developed as part of this research to readily control its outlet organic vapor concentration as the entire inlet gas stream passes through the CAD system. This bench-scale system adsorbed organic vapor from a gas stream and simultaneously heated the adsorbent using direct electrothermal energy to desorb the organic vapor at user-selected set-point outlet concentrations. CAD achieved a high degree of concentration stabilization with a mean relative deviation between set-point concentration and measured outlet vapor concentration of 0.3 % to 0.4 %. The CAD system was also evaluated to treat a humid
gas stream (inlet relative humidity = 85%) that contained a variable organic vapor concentration. CAD operated successfully at high inlet relative humidity conditions because the water vapor did not adsorb but penetrated through the adsorbent because of local warming of the adsorbent.

Computational fluid dynamics was used for the first time to model the three-dimensional (3-D) pressure drop, flow patterns, and heat transfer in an adsorption vessel with annular cartridges of ACFC. It was demonstrated that pressure drop and velocity contours are very uniform (e.g., within 5%) in the porous zones of the ACFC cartridges within the vessel. The main pressure drop across the vessel is due to the ACFC cartridges. It was also demonstrated that electrothermal heating is much more energy efficient than heating with hot inert gas such as air. These results support the use of 1-D or 2-D modeling regarding mass and energy transfer in the ACFC while achieving sufficient accuracy.

A fundamental mathematical model for simulation of ESA was also developed and evaluated. The model consists of: a) material balances for organic vapors in the adsorption vessel and b) energy balances for the adsorbent, carrier gas, vapor, and fittings. The model predicts outlet vapor concentrations, temperature profiles, power requirements, voltage requirements, and current requirements for ESA desorption cycles. The model is very helpful in the initial stages of design of an ESA system to reduce cost and time and to more effectively evaluate experimental results pertaining to energy and material balances.

Future work that should occur includes the development and testing of VaPRRS, SST, and CAD at the full-scale. Results from these tests can then be used to compare these technologies to existing air quality control technologies and to evaluate these new systems under more realistic field conditions that exist in the laboratory. CFD simulations can also be developed and implemented to consider mass transfer within the adsorption vessels and to consider new adsorbent geometries, such as pleated cartridges in rectangular enclosures. ESA VaPRRS/SST/CAD should also be developed for indoor air quality control applications. Such technologies have the potential to remove particulate
matter, organic gases, and biological materials from indoor air streams.
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1. INTRODUCTION

1.1. Hazardous Air Pollutant/Volatile Organic Compound Emissions

United States Environmental Protection Agency (USEPA) reported that $1.6 \times 10^{10}$ kg of VOCs and $5.7 \times 10^8$ kg of hazardous air pollutants HAPs were emitted to the atmosphere from anthropogenic sources during 2001 and 2002, respectively (USEPA, 2004a; 2004b). USEPA also reported that $1.9 \times 10^{10}$ kg of volatile organic compounds (VOCs) were released to the atmosphere during 2000 (USEPA, 2004c). Many of these compounds are emitted into the atmosphere each year by industrial sources such as surface coating, printing, and cleaning operations. A reduction in the quantity of these emissions that are emitted into the atmosphere can be achieved by using a variety of methods, including process modifications, destructive techniques, and recovery techniques. Adsorption with regeneration and liquification of the vapor is an example of a technology that can meet USEPA’s emission standards while allowing for recovery and reuse of the material removed from the gas stream.

1.2. Green Chemistry & Sustainability

The concept of sustainability according to the “Brundtland” report is "development that meets the needs of the present without compromising the ability of further generations to meet their own needs” (World Commission on Environment and Development, 1987). Strong interest in achieving sustainability encourages the modification of consumption patterns to allow for continued economic development. The concept of sustainability focuses on the preservation of our natural resources for future generations. A technology that involves a process to be considered sustainable should meet requirements such as: the waste must be minimized and all the by-products from manufacturing and consumption should be recovered and reused over time; the inevitable wastes should have minimal impacts on the environment and should fit into established remediation programs; the energy that drives the process should be minimal, while making use of all possible engineering achievements that promote maximum efficiency; and the energy should come from non-fossil sources whenever possible (Roberts, 1994).
Before the promulgation of Federal regulations, it was common to emit organic vapors directly to the atmosphere. USEPA was formed in 1970. Since then environmental concerns have been acknowledged by setting pollutant emission standards and controlling the release of select organic vapors to the atmosphere through environmental laws. Pollution prevention prevents the formation of wastes rather than treating of the wastes. One type of pollution prevention is Green Chemistry. Green Chemistry, or environmentally benign chemistry, is the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances (Anastas and Warner, 1998). Green Chemistry is based on 12 principles such as designing safer chemicals, real-time analysis for pollution prevention, auxiliary solvents should be innocuous or avoided whenever possible, and energy usage should be minimized. Achieving all principles of Green Chemistry is a tremendous challenge. For example, substitution of hazardous solvents with more benign materials is not always easy to accomplish. Many paint applications have strict requirements that can’t attained with available material substitutes. It is necessary to have an energy-efficient technology that will allow capture and recovery or destruction of HAPs and other vapors until the time that alternative solvents are developed that are as effective as existing solvents, but are environmentally benign.

1.3. Control Methods

Control methods include process modifications, destructive techniques, and recovery techniques as described in the next sections.

1.3.1. Process Modifications

Substitution of raw materials or modification of operating conditions and equipment is an ideal way to reduce the emissions of HAPs into the atmosphere. Unfortunately process modification is not always possible due to technological or economical limitations.

1.3.2. Destructive Techniques

Destructive techniques such as thermal, catalytic, and biological oxidation are often
selected because they offer the lowest-cost solution for compliance with environmental regulations. An oxidizer burns the organic compounds to produce less harmful compounds such as CO\(_2\) and H\(_2\)O. The nominal operating range for thermal oxidizers is 700\(^\circ\)C to 1200\(^\circ\)C, while catalytic oxidizers operate at temperatures between 340\(^\circ\)C and 590\(^\circ\)C by using a catalyst to reduce the activation energies of the combustion reactions (Altwicker et al., 1999; Hunter and Oyama, 2000). Thermal oxidizers can have very high conversion efficiencies (> 99%). However, oxidation is an expensive option to control dilute VOC content gas streams, as additional auxiliary fuel is needed to achieve complete combustion and additional CO\(_2\) is emitted into the atmosphere. Moreover, oxidation of halogenated compounds results in the formation of halo-acids such as hydrochloric acid (HCl).

Another option is to use gas-phase biofilters that allow microorganisms to aerobically metabolize the gaseous contaminants. The microbes form a biofilm on a support media, typically a natural cellulose-based material such as compost or wood chips. Advantages of biofiltration include vapor removal efficiencies up to 90% and low operating costs. Biofilters are suitable for gas streams with pollutant concentrations in the tens to hundreds of ppmv. However, biofiltration is not suitable for treating gas streams with highly variable vapor concentrations or gas streams emitted from batch systems in which products change daily or weekly because the microbes are sensitive to significant changes in the types and/or concentration of pollutants and can be killed by sudden changes. Adequate moisture level and relatively constant temperature are also needed for proper operation of biofiltration (Altwicker et al., 1999; Hunter and Oyama, 2000; Li et al., 2005).

1.3.3. Recovery Techniques

Recovery techniques such as condensation, membrane separation, absorption, and adsorption are preferred where possible, since they conserve resources, do not generate greenhouse gasses, and save money by recovering a valuable product.

Condensation is typically achieved by lowering the temperature below the dew point
of the feed gas while keeping the total pressure constant (Altwicker et al., 1999). Cooling capacity can be provided by chilled water, mechanical refrigeration, or cryogenic fluids, depending on the relative pressure of pollutant in the gas stream. Condensation is most efficient for organic vapors with boiling points higher than 38°C (Khan and Ghoshal, 2000). Condensation allows the recovery and reuse of organic vapors. Condensation of organic vapors is suitable for relatively high-concentration gas streams (more than 0.5% by volume), otherwise a concentration process is required prior to condensation for dilute gas streams and there are numerous moving parts and large changes in pressure needed to achieve the desired cooling capacity.

Membrane separation technology provides a partial pressure gradient across a semi-permeable membrane for either the pollutant or the carrier gas to pass through. Membrane separation systems can achieve removal efficiencies as high as 90 to 99.99%. Membranes must have material and mechanical compatibilities with the gas stream that needs to be treated. A common limitation of membrane separation systems is the possibility of membrane fouling due to the presence of particles or oily compounds. As such, a pretreatment process might be needed to avoid membrane clogging (Hunter and Oyama, 2000). The capital cost and pressure drop of membrane separation make this technology impractical for many air quality control applications that contain dilute organic vapors.

Absorption or “wet scrubbing” consists of transferring the pollutants from a carrier gas into a contacting liquid in which the pollutant is soluble. The driving force for absorption is the difference in the pollutant’s vapor pressure (or activity) between the gas and liquid phases. The advantage of absorption is its flexibility and ability to handle a large range of gas flow rates (Altwicker et al., 1999). The major disadvantage of absorption is that the absorbed pollutant then needs to be separated from the liquid stream, which can be energy intensive (Altwicker et al., 1999; Hunter and Oyama, 2000).

Adsorption removes pollutants from gas streams by contacting the gas stream with an interface, usually a gas–solid interface. Adsorption is used for organic vapor control when the vapor concentration is at low (20 ppmv) to medium (20,000 ppmv) levels,
a stringent outlet concentration is to be met, and/or recovery of the vapor is desired (USEPA, 2002).

### 1.4. Adsorbents

Adsorbents commonly used in air pollution control devices are granular activated carbon (GAC), activated carbon fiber cloth (ACFC), silica gel, and zeolites. Physical properties of these adsorbents are provided in Table 1-1.

<table>
<thead>
<tr>
<th>Adsorbent</th>
<th>Nominal surface area (m²/g)</th>
<th>Nominal micropore volume (cm³/g)</th>
<th>Nominal pore width (nm)</th>
<th>Nominal external diameter (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GAC</td>
<td>1,200</td>
<td>0.44</td>
<td>2-4</td>
<td>1,000-7,000</td>
</tr>
<tr>
<td>ACFC</td>
<td>800-1,900</td>
<td>0.35-0.9</td>
<td>0.6-0.9</td>
<td>12</td>
</tr>
<tr>
<td>Silica gel</td>
<td>250-900</td>
<td>0.45-1</td>
<td>2-24</td>
<td>&gt; 1,000</td>
</tr>
<tr>
<td>Zeolites</td>
<td>1-20</td>
<td>0.3</td>
<td>1.0</td>
<td>&gt; 1,000</td>
</tr>
</tbody>
</table>

Table 1-1. Select Properties of Typical Adsorbents

*a Do, 1998  \b Lo, 2002

Activated carbons are the most commonly used adsorbent for removal of organic vapors from gas streams. Activated carbons are amorphous carbon-based materials with large surface areas, commonly have microporous structure, and provide high adsorption capacities (Bansal et al. 1988). They have large surface areas as a result of an activation process in which the carbonaceous material is oxidized with air, steam or CO₂ at high temperatures (Bansal et al., 1988). The raw materials for the manufacture of activated carbons can be natural and synthetic such as peat, coal, lignite, wood, coconut shells and polymers (Bansal et al., 1988), waste tires (Lehmann et al., 1998) and resins (Hayes 1981). Activated carbons are produced in different forms such as powders and granules (Bansal et al., 1988), monoliths (Yu et al., 2002), fibers, and fiber clothes (Hayes 1981).

Powdered activated carbons (PACs) are produced mainly from sawdust using chemical methods (Bansal et al., 1988). An average particle diameter of 15 µm to 25 µm
provides the activated carbon large external surfaces with small diffusion distances (Bansal et al., 1988) that make them particularly useful in water quality applications.

Granular activated carbon (GAC) is commonly used in the adsorption of gases/vapors because of they allow for fast diffusion rates of gases/vapors. GAC can be prepared by physical activation using carbonaceous materials such as select coals, woods, coconut shells, petroleum products, heavy oils, synthetic and natural rubbers (Bansal et al., 1988), and waste tires (Lehmann et al., 1998). GAC granules are larger than PAC which gives GAC smaller external surface per unit volume as compared to PAC. The GAC granules are produced at different sizes for different applications. For instance, for deodorization filters the diameter of GAC range from 1 mm to 3 mm, and for industrial adsorbers the granular diameter can be 4 mm to 7 mm in diameter (Smísek and Cerný, 1970). Smaller GAC granules cause larger pressure drop in an adsorption vessel (Bansal et al., 1988).

Activated carbon monolith (ACM) is prepared from activated charcoal powder and a binder to form the monolith. ACM has shown similar adsorption capacities of VOCs as commercial granular adsorbents (Yu et al., 2002; Luo et al., 2006).

Activated carbon fibers (ACFs) can be made from Novoloid, pitch, cellulose, rayon, polyacrylonitrile and saran (Hayes 1981; Lo 2000). ACFs are shapeable and can be formed as activated carbon fiber paper, fiber felt, and cloth (ACFC). ACFC is a novel adsorbent that has recently been shown to be an effective adsorbent to capture and recover organic vapors from gas streams at a wide range of concentrations (Sullivan et al., 2004a; Ramirez et al., 2004). ACFC is synthesized chemically and pore size can be carefully controlled. Novoloid ACFC is 95% carbon after carbonization and activation, with the balance containing hydrogen, oxygen, and nitrogen (Lordgooei, 1999). The adsorbent’s electrical resistivity also allows for rapid heating and regeneration of the adsorbent and recovery of the adsorbate as a liquid (Sullivan et al., 2004a). The adsorbent is free of impurities that can lead to chemical reactions such as fires in the adsorbent (Zerbonia et al., 2000; Hayes Jr. and Sakai, 2001).

ACFC is microporous with a narrow pore width distribution. The micropores exist on
the fiber surface and throughout the fiber (Economy et al., 1995; Daley et al., 1999). The adsorbent has extremely small pores with 96 % of its surface area in pores with widths < 10 Å. The fabric is also very porous with total pore volume and micropore volume of 0.8 and 0.75 cm³/g, respectively, making the material an excellent adsorbent for organic vapor capture. A typical surface area of ACFC is 2,000 m²/g, but can be as high as 2,500 m²/g (Hayes, 1981). A typical fiber diameter is 10 μm (Mays, 1999), while the average micropore width is typically less than 20 Å (Hsi, 2000). ACFs allow for more ready access of the adsorbate to the pores (Mays, 1999) and more rapid heat transfer because the dimension of the fibers is orders of magnitude smaller than the dimension of granules. The uniform distribution of pores and pore widths allows for ACFs to be tailor-made for a particular application.

Another advantage of ACFC is its electric conductivity. ACFC can conduct electricity because it consists of closely woven yarns allowing for close contact between the fibers within the yarns. This unique property of ACFC allows for electrothermal regeneration by means of electrical resistance heating (Joule heating) (Lordgooei et al., 1996).

ACFCs that were used in this research were ACFC-15 and ACFC-20. Physical properties of these adsorbents are provided in Table 1-2 (Lo, 2002).

BET (Brunauer-Emmett-Teller) surface area is surface area of an adsorbent measured by the BET technique. BET is a generalization of Langmuir theory (a theory for monolayer molecular adsorption) to multilayer adsorption. BET surface area is one important factor in determining the adsorption capacity of activated carbon. BET surface area of ACC-20 is 20% more than that of ACC-15.

Pore width and pore volume are also important parameters in characterizing activated carbon because adsorption potentials influence adsorption capacity which depend strongly on pore width. Also, the presence of high micropore volume and surface area allows for a large number of adsorption sites, and a relatively large pore network to facilitate transport of adsorbate molecules into the interior of the adsorbent (Do, 1998). Micropore volume comprises more than 90% of total pore volume for both ACC-15 and
ACC-20. However, ACC-20 has 20% more micropore volume than ACC-15. Both adsorbent have average micropore width of 6.9 Å.

Areal density is defined as the mass of the ACFC sample divided by the bulk cross-sectional area (the product of the width and length of the ACFC sample) of that sample. Areal density is useful in calculating the length of cloth needed for specific applications knowing the required mass of ACFC based on its adsorption capacity. Areal density of ACFC-20 is 8% lower than that of ACFC-15.

The porosity of ACFCs is a function of the void volume between the fibers and between the yarns, which are fibers spun together in a bundle. This is different than porosity of the ACFs which is a function of the total pore volume inside the fibers. The porosity of ACFCs affects the gas flow pattern and pressure drop in the ACFCs, while porosity of fibers affects the adsorption capacity of ACFCs.
### Table 1-2. Physical Properties of ACC-5092-15 and ACC-5092-20

<table>
<thead>
<tr>
<th>ACFC</th>
<th>BET Surface Area (m²/g)</th>
<th>Total Pore Volume (cm³/g)</th>
<th>Micro-pore Volume (cm³/g)</th>
<th>Pore Volume Micro-porosity (%)</th>
<th>Average Micropore Width (Å)</th>
<th>Envelope Density (g/cm³)</th>
<th>Areal Density (g/m²)</th>
<th>Porosity (%)</th>
<th>Electrical resistivity (ohm·m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACC-5092-15</td>
<td>1322</td>
<td>0.658</td>
<td>0.621</td>
<td>94.4</td>
<td>6.9</td>
<td>0.91</td>
<td>166</td>
<td>N/A^a</td>
<td>-2 × 10⁻⁵T + 0.0113^b</td>
</tr>
<tr>
<td>ACC-5092-20</td>
<td>1604</td>
<td>0.803</td>
<td>0.746</td>
<td>92.9</td>
<td>6.9</td>
<td>0.80</td>
<td>152</td>
<td>51.3</td>
<td>-2 × 10⁻⁵T + 0.0119^b</td>
</tr>
</tbody>
</table>

^aN/A = not available  
^bT = temperature (K)
Envelope density is the density of porous fibers (mass of fibers divided by volume of fibers). Since ACC-20 is more porous than ACC-15 it has lower envelope density. Envelope density of fibers and porosity of ACFC determine the thickness of a cartridge made from ACFC.

Electrical resistivity is an intrinsic parameter for characterizing the electrical property of ACFCs. This parameter is dependent on the temperature, precursor and weaving pattern of the ACFC samples, and is independent of the sample geometry (Subrenat et al., 2001). The resistivity generally increases with increasing level of activation. This might be due to increased amount of material removed from the sample with increasing levels of activation, which results in increased porosity of the adsorbent and hence decreased cross-section available for current to flow through the adsorbent. Electrical resistivity is an important property of ACFC that makes it suitable for resistive heating in which the adsorbent is treated as an electrical resistor in a circuit while applying an electric potential across it. This is called direct electrothermal regeneration. This electrical property of ACFC allows the adsorbent to be heated up within seconds to minutes during electrothermal desorption. This is the basis for electrothermal swing adsorption (ESA) technology.

Physical and chemical properties of ACFCs may be modified in order to tailor the adsorption and regeneration properties of activated carbon for specific air quality applications. It is possible to have more selective ACFC by changing the amount of chemical functional groups on the surface of ACFC. For instance, adding oxygen functional groups to ACFC will enhance the adsorption of water vapor (Dimotakis et al., 1995a; Dimotakis et al., 1995b), basic compounds such as ammonia, and polar compounds such as acetone (Mangun et al., 1999). Similarly, treating ACFC with ammonia will enhance its adsorption capacity for acidic vapors such as hydrochloric acid (HCl) and sulfur dioxide (SO₂) (Mangun et al., 2001a; Mangun et al., 2001b). H₂ treatment will make ACFC more hydrophobic which is desirable for treating humid gas streams and such treatment modifies the microwave adsorption properties of the ACFC (Hashisho et al., 2009; Sullivan et al., 2007).
Adsorbents are typically used in a cyclical pattern to allow for alternating adsorption and regeneration cycles. However, repetitive adsorption and regeneration cycles can ultimately reduce the adsorbents chemical and structural integrity causing attrition and reductions in the adsorbent’s adsorption capacity. Since ESA technology has not been utilized over lifetimes of years with a commercialized system, there are no data available on extended life times (e.g., years) of ACFCs.

Trade-offs/limitations of ACFC include the high cost of ACFC ($600/kg) when compared to GAC ($2/kg). Also, ACFC is composed of carbon that thermally decomposes in air at 300 °C (Puri et al., 1964; Barton et al., 1973 and 1978). Another aspect of ACFC is that it is the form of a cloth that does not lend itself to for use in fluidized beds or induct injection that is possible with GAC.

1.5. Regeneration Techniques

Regeneration is a process of removing adsorbate from an adsorbent. Regeneration of an adsorbent is accomplished by reducing the total pressure (pressure swing), increasing the temperature (thermal/temperature swing), reducing the adsorbate’s partial pressure (purge gas stripping), and use of a competitive adsorbate (displacement desorption).

Pressure Swing Adsorption (PSA) is a gas separation process in which the adsorbent is regenerated by reducing the total pressure within the vessel containing the adsorbent and thereby reducing the partial pressure of the adsorbate(s). PSA is commonly used for separation of oxygen from air. However, PSA is also used for capture and recovery of organic vapors at bulk gasoline terminals.

Thermal/temperature-swing adsorption (TSA) typically includes heating of adsorbent with steam, inert purge gas (Figure 1-1a), close-proximity resistive elements, or microwaves. Direct electrothermal regeneration (electrothermal swing adsorption or ESA) is an alternative technique that treats the adsorbent as a resistor in a circuit while applying an electric potential across it (Lordgooei, 1999, Sullivan, 2003; Rood et al., 2003a, 2003b, 2004, 2009; Kaldate et al., 2003a & 2003d; Ramirez, et al., 2005 & 2006; Vidal et al., 2006, Thurston et al., 2009), as it is demonstrated in Figure 1-1b.
Figure 1-1. Regeneration of the ACFC by Thermal Swing Adsorption (a) vs. Electrothermal Swing Adsorption (b)

ESA technology can use ACFC and allow rapid adsorption and desorption with in-vessel condensation to recover the organic vapor as a liquid. The system typically consists of two adsorption vessels. Each vessel typically contains two or more annular cartridges that are oriented vertically in the vessel. During the adsorption cycle, the gas stream enters the inside of the cartridges, passes through these cartridges and into the open vessel, and finally exits the vessel. There have been other designs with different flow configurations as well (Lordgooei, 1999, Sullivan et al., 2001, Sullivan et al., 2004a, Dombrowski et al., 2004). For instance, two cartridges in series (the gas stream
enters the inside of one cartridge, passes through it to the open vessel, then passes from the outside of the second cartridge to its inside, and then finally exists the vessel from the inside of the second cartridge). The advantage of this configuration is that the gas stream passes through more layers of ACFC and as a result of that, effectively reduces the non-uniformity (i.e. tightly woven fabric) of the ACFC cartridges. However, if cartridges are prepared carefully, this configuration has no advantages. Furthermore, pressure drop is higher because gas passes through more layers of adsorbent. Regeneration of the ACFC occurs by direct electrothermal heating of the adsorbent while passing N₂ through the vessel. This technology does not require additional unit operations to recover the organic compound because the organic vapor rapidly condenses in the vessel inner wall at ambient temperature, saves energy and decreases costs in comparison to other conventional desorption technologies (Sullivan et al., 2004a; Dombrowski et al., 2004; Sullivan, 2003).

ACFC that has adsorbed HAPs/VOCs is regenerated by Vapor Phase Removal and Recovery System (VaPRRS, Lordgoeei et al., 1999; Rood et al., 2002; Sullivan et al., 2004a and 2004b; Hashisho, 2007) allowing for adsorption and then regeneration to recover valuable HAPs/VOCs as liquids.

The unique aspects of ESA are:

- ESA has very high energy efficiency: Unlike common thermal swing adsorption (TSA) technologies that use a hot carrier gas or steam to regenerate the adsorption bed, applied power and carrier gas flow rate are controlled separately.

- ESA is simple, with no moving parts or ancillary equipment except for valves to direct fluid flow. Also, adsorption and regeneration occur inside the same adsorption vessel.

- The captured material is not contaminated: Unlike common steam generation systems, water is not introduced to the system that contaminates the recovered material.

Cost analyses have shown that VaPRRS technology is economically competitive with existing technologies (Kaldate et al., 2005, 2006). In this analysis two other main
competing technologies, granular activated carbon (GAC) adsorption and thermal incinerator (TI) were considered along with optimal design of 4,000 ft³/min ESA device for MEK concentration of 525 ppmv using ACFC-15 as an adsorbent (Kaldate, 2005).

ESA with ACFC offers the following improvements over existing technologies:

- ACFC eliminates unwanted chemical reactions and fires that occur with traditional granular activated carbon because ACFC is ash-free while GAC contains ash that is associated with unwanted chemical reactions and fire (Zerbonia et al., 2000).
- Ancillary devices and water injection that are used with existing steam and hot air regeneration technologies are eliminated.
- Simple and efficient power application to the ACFC minimizes energy losses to the vessel and ancillary equipment that occur with existing technologies.
- Independent control of gas flow rate and regeneration power provides robust control of low-flow-rate effluent gas streams containing vapor concentration ranging between liquid for recovery and reuse (VaPRRS).

Energy/liquid mass recovered for three organic vapors (methyl propyl ketone (MPK), MEK, and hexane, 69°C < boiling point < 102°C) is reported between 4 kJ/g and 8 kJ/g for bench-scale tests (Dombrowski et al., 2004) and between 5.7 kJ/g and 10.7 kJ/g for three organic vapors (MEK, MPK, toluene, 69°C < boiling point < 111°C) for pilot-scale ESA results (Ramirez, 2005). However, the steam to solvent mass ratio for steam regeneration ranges from 2/1 to 8/1 for an optimized steam regeneration system to recover an unspecified solvent (Walas, 1990). Such steam to solvent ratio is equivalent to 5 to 18 kJ/g of solvent recovered assuming 100% recovery of the solvent. Energy requirements for steam regeneration were also reported to range between 9 kJ/g and 39 kJ/g for two organic vapors (toluene, perchloroethylene, 111°C < boiling point < 121°C) (Danielson, 1973, Noll 1999). It is also important to note that the energy requirements for steam regeneration do not appear to include the energy to dry the adsorbent after regeneration that is not needed for ESA. The ESA system is also flexible to design and
implement in a wide range of configurations due to the resistivity and shapeability of the fabric.

Biofiltration and oxidation are attractive HAP/VOC disposal techniques because they can convert organic vapors into carbon dioxide, water vapor, and/or biomass. However, as discussed before fluctuations in concentration of the vapor and high gas flow rates of the gas stream to be treated makes it challenging for biofilters and oxidizers to operate efficiently. For instance, high organic vapor concentration can be toxic while low concentrations can cause starvation of microorganisms in a biofilter, which results in reduced biomass and removal efficiency of the HAPs/VOCs. Similarly, low organic vapor concentrations result in increasing the consumption of auxiliary fuel necessary to sustain the appropriate temperature when using oxidation. Designing a biofilter or an oxidizer to meet the maximum concentration of the vapor in the gas stream and at the total gas flow rate that is generated by the source(s) results in a larger control device than is necessary to treat the average vapor concentration in the gas stream. Hence there is a need to dampen the fluctuations in vapor concentration in gas streams and reduce the total gas flow rates that are treated by biofiltration or oxidation to allow for a more reliable, efficient and cost-effective control system. Adsorption has been used to concentrate organic vapors upstream of oxidizers (Chang et al., 2003; Mitsuma, 1998). A rotating honeycomb of silica zeolite monolith was used as a concentrator upstream of a thermal oxidizer to increase cyclohexane vapor concentration by 10 times during hot air desorption (Mitsuma, 1998). Another honeycomb zeolite concentrator successfully increased the concentration of semiconductor production related VOCs (e.g., isopropyl alcohol, acetone, propylene glycol methyl ether, and propylene glycol monomethyl ether acetate) by 6.5 to 19.5 times (Chang et al., 2003). However, in both systems, there was no active control of the vapor concentration during the regeneration cycle, and the resulting vapor concentration was not controlled separately from the gas flow rate because the energy used to desorb the vapor was provided by the hot air carrier gas. It was reported that the ratio of vapor concentrations between the desorption and adsorption cycles was determined by the ratio of gas flow rate during those cycles (Chang et al., 2003).
In ESA regeneration power is readily controlled independent of inlet gas flow rate. Unlike existing technologies, independent control of power and gas flow rate allow for careful control of the adsorbent’s temperature and the resulting outlet vapor concentration.

1.6. Objectives, Contributions, Significance, and Overall Research Methodology

The main objectives, significance, and methodology for this research are discussed in the following sections.

1.6.1. Objectives

The objectives of this research are:

- Build up an automated bench-scale VaPRRS system and perform sequentially designed sets of laboratory experiments that are used to:
  - Identify factors that can increase the adsorbate liquid recovery with low energy costs by Kaldate (2005)
  - Develop a scale-up model of ESA-VaPRRS by Kaldate (2005) to find optimal values of decision variables
  - Compare the bench-scale VaPRRS to a pilot-scale VaPRRS

- Modify the bench-scale ESA-VaPRRS to a Steady-State Tracking (SST) and Concomitant Adsorption Desorption (CAD) systems to:
  - Investigate and demonstrate ESA-SST for three organic compounds (methyl ethyl ketone, acetone, and toluene) at low and high concentrations in batch mode
  - Investigate and demonstrate ESA-SST for dynamic set-point conditions while gas flow rate of gas stream changes during the operation
  - Demonstrate cyclic operation of ESA-SST to demonstrate such capability
without operator intervention

- Demonstrate and characterize the operation of CAD for dry and humid gas stream

- Model the three-dimensional (3-D) pressure drop, flow patterns, and heat transfer in an adsorption vessel with annular cartridges of ACFC by using computational fluid dynamics (CFD)

- Develop and evaluate a comprehensive mathematical model to simulate VaPRRS and ESA-SST during their regeneration cycles

1.6.2. Contributions

Contributions that are provided by this research are described below:

- The most efficient engineering parameters for the next generation of VaPRRS were identified in collaboration with Kaldate (2005). Specific contributions by this research included the designing and building of an automated bench-scale VaPRRS and performing experimental tests to provide input data to analytical methods developed and implemented by Kaldate (2005) to optimize VaPRRS. These input data were important to quantify engineering parameters that were not previously available and needed by Kaldate (2005) to complete the analysis.

- New concentration controlled desorption systems (SST and CAD) were conceptually developed, designed, built and demonstrated experimentally to operate over a wide range of conditions. These new systems were designed to provide more stable outlet organic vapor concentrations with independent control of heating and gas flow rate during desorption cycles.

- The fluid flow patterns were characterized inside the ESA adsorption vessel using CFD simulations to demonstrate uniform distributions of pressure drop and gas velocities inside the adsorbent and to justify the use of 1-dimensional (1-D) simulations which are computationally less intensive than 3-D simulations.
A mathematical model was developed to simulate heat and mass transfer in an ESA system for use in the early stage of design of a full-scale ESA system to reduce cost and time associated with experimental testing over a wide range of conditions.

The experimental and modeling results from this work made overall contributions to the larger picture of environmental impact such as energy consumption during the regeneration of ACFC. Results provided here were used by Kaldate (2005) to provide a scaled-up model and optimal design of an ESA-VaPRRS system with lower energy consumption. Other contributions to reducing environmental impact include reducing the consumption of adsorbates that are recovered with VaPRRS instead of destroyed (i.e., thermal oxidation/biofiltration), using less resources to dispose of adsorbates that do not warrant recovery with the use of SST/CAD pre-treatment, and reducing the environmental impact of disposal activities for the unrecovered adsorbate.

1.6.3. Significance

This research is significant because:

- VaPRRS experimental data from this work provided important inputs to analytical methods developed by Kaldate (2005) to identify significant factors contributing to energy consumption of VaPRRS. Based on the experimental data provided in this research, a full-scale model was developed by Kaldate (2005) and was used to determine optimal values of decision variables (Kaldate, 2005). Comparison of the bench-scale VaPRRS and the existing pilot–scale VaPRRS confirmed that this newly developed ESA technology can be improved and used more efficiently for the removal and recovery of organic vapors.

- ESA-SST system was developed and tested in this research to have three main advantages over existing technologies:
  - Lower energy consumption,
More stable outlet concentration of the organic vapors during adsorbent regeneration cycles

Ability to independently control the heating source and gas flow rate over a wide range of conditions

- 3-D computational fluid dynamics (CFD) simulation of fluid flow and heat transfer demonstrated quantitatively that pressure drop and gas velocity distributions are uniform inside the ACFC cartridges and consequently justified the use of 1-D modeling which is computationally less intensive than 3-D simulations. Such 3-D simulations also demonstrated quantitatively that electrothermal heating is more efficient than heating by hot air.

- The numerical modeling of heat and mass transfer that was developed in this work and compared to experimental results is now available for the early stages of development and design to reduce cost and time without spending an extensive amount of experimental resources.

1.6.4. Methodology

The overall methodology of this research is described in Figure 1-2. An automated bench-scale ESA system is built to study the capture of organic vapors from gas streams and recover them as a liquid stream (VaPRRS). This system will also be used to desorb the vapors at a controlled constant concentration (ESA-SST), which can then be efficiently treated with a biofilter or a thermal oxidizer. Results from a comprehensive mathematical model to simulate the desorption of organic compounds as VaPRRS or as ESA-SST will also be developed and compared to experimental results. Results from the experiments and simulations will be used to evaluate these technologies and compare them with other existing technologies.
1.6.4.1. Automatic Bench-Scale VaPRRS System

The bench-scale VaPRRS system consists of a vapor generation system, two adsorption/regeneration vessels, organic vapor detector, and a data acquisition/instrumentation control system. The vapor generator consists of a source of filtered compressed air, a custom silica gel adsorber, a mass flow controller, and a syringe pump. The adsorption/regeneration vessels consist of an aluminum or stainless steel cylinder, a conical base, and a top plate. The top plate is made of Teflon to ensure electrical isolation of the ACFC during electrothermal regeneration of the ACFC. Two or four annular cartridges of ACFC will be located vertically in the cylindrical portion of the vessel. Adsorption and desorption cycles will be controlled by a fully automatic microprocessor-based measurement and control.

1.6.4.2. Modification of VaPRRS to ESA-SST System

VaPRRS is modified to allow for desorption of organic vapors from the ACFC at carefully controlled concentrations, so that it can be tested as an efficient means to feed
organic vapors to a biofilter or an oxidizer. The concentration of organic vapor at the vessel’s outlet during the regeneration cycle will be controlled with the use of proportional-integral-derivative (PID) control of the electrical power applied to the ACFC to achieve the desired set-point concentrations.

1.6.4.3. Fluid flow and Heat Transfer Simulation

Computational fluid dynamics (CFD) analysis will be completed by using software package, FLUENT, to investigate the gas flow pattern inside the adsorption vessel and cartridges. CFD simulation of unsteady-state heating of the cartridges in the vessel will also be performed by solving fluid flow and heat transfer equations using FLUENT.

1.6.4.4. Develop and Evaluate a Comprehensive Mathematical Model to Simulate VaPRRS and ESA-SST

Mathematical model simulated mass and heat transfer in the ESA systems will be developed. The model will be based on one-dimensional fundamental equations of transient mass and energy transfer within the system. Results from the simulations will be compared to independently obtained experimental data.

Experimental analyses can be expensive and time consuming, while computer simulations can cost less and require less time to provide valuable insight about the design and optimization of the ESA systems. The models that will be developed as part of this research can be used to investigate the contribution of different parameters to the consumption of energy during the regeneration of the ACFC and can be integrated with optimization tools to optimize the system. Simulations are also very useful for preliminary design of VaPRRS and ESA-SST systems.
2. RESEARCH METHODOLOGY

2.1. ESA-Experimental Setup

The bench-scale experimental equipment used in this research consists of a dual vessel automated ESA system (Figure 2-1). In order to investigate the effect of heat transfer properties of adsorption vessel on the liquid recovery and energy consumption, one vessel is made of aluminum and the other one is made of stainless steel 316.

![Figure 2-1. Bench-Scale Electrothermal Swing Adsorption System](image)

The bottom of each vessel is conical to allow liquid VOC/HAP to readily drain liquid from the vessels. The external diameter of each vessel is 15.2 cm with a wall thickness of 0.95 cm. The cylindrical and conical portions of the vessel were 23.5 cm and 8.2 cm, tall, respectively. Top plates on each vessel are made of Teflon to ensure electrical isolation during electrothermal regeneration of the adsorbent. Teflon is also inert and is a good choice for most solvents. Two or four annular cartridges of ACFC (Figure 2-2) are utilized in each vessel. Temperatures of the cartridges and external wall of the vessel were measured with Type K thermocouples (0.0254 cm diameter, Omega Inc.) that were located at the vertical center of the cartridges and the cylindrical portion of the vessel’s external wall.
The vapor generator consisted of a source of filtered compressed air, a custom silica
gel adsorber, a mass flow controller (Aalborg, Model GFC571S), and a syringe pump
(KD Scientific, Model 200) with 100 ml syringe (Hamilton). During the adsorption time,

![Stainless steel tube]( Figure 2-2. ACFC Cartridge

A constant concentration of VOC to the inlet of the vessel is obtained by evaporating
liquid VOC into a dried air stream. A syringe pump (KD Scientific, model 200) and 100
ml syringe (Hamilton Inc.) is used to supply a constant flow rate of liquid HAP/VOC to
the carrier gas stream. A mass flow controller (Aalborg, Model GFC571S) controls the
flow rate of the carrier gas (i.e., air) up to 200 slpm (s = standard temperature and
pressure, STP = 70°F, 101 kPa). A material balance for the HAP/VOC and air stream was
used to determine the injection rate for the liquid HAP/VOC and its resulting
concentration in the air stream.

The measured electrical power applied to the cartridges was determined with root
mean square (RMS) voltage and current values obtained from the fully automatic
microprocessor-based measurement and control system (National Instruments Inc.) using LabView software. There was no operator intervention of the data acquisition and control system during the adsorption or regeneration tests.

2.1.1. ESA-VaPRRS

A schematic of the ESA-VaPRRS setup is shown in Figure 2-3. During the adsorption cycle, the gas stream enters one adsorption vessel, passes through the cartridges, and then exits from top of the vessel (Figure 2-4). The air flow rate was kept at 100 slpm (STP = 0°C, 101 kPa) during all absorption tests. The gas stream is switched between vessels when the outlet concentration reaches 5% of the inlet value. Regeneration of the ACFC occurs by direct electrothermal heating of the adsorbent while passing nitrogen through the cartridges in the reverse direction.

Figure 2-3. Schematic of Electrothermal Swing Adsorption System
As previously mentioned, this system is operated by a fully automatic microprocessor-based process control system with no operator intervention. The microprocessor switches the gas stream from the saturated vessel to the stand-by vessel, the vessel with the saturated ACFC is purged with nitrogen at 5 slpm for 3 minutes (=15 liters; that is more than 4 times the volume of empty vessel which is about 3.5 liters) to remove oxygen from the vessel, the saturated ACFC cartridges are then regenerated electrothermally while nitrogen flows through the cartridges and vessel at a constant flow rate, liquid VOC/HAP flows from the regenerated vessel, cartridges are cooled, and vessel is then placed in stand-by mode. The flow rate of nitrogen is kept constant by using mass flow controllers (Tylan, FC-260KZ, FC-280SAKZ). In order to increase the overall pollutant recovery to ~100%, the nitrogen is recycled to the inlet gas stream of the second vessel. Concentrations of VOC in the exhaust gas and in the recycle line are measured by using a photo ionization detector (PID*, RAE Systems Inc., PDM-10A), and a flame ionization detector (FID, Baseline Series 8800), respectively.

Figure 2-4. Gas Flow Path During Adsorption and Regeneration

![Diagram of gas flow path during adsorption and regeneration](image)
2.1.2. ESA-SST

A schematic of the ESA-SST setup is shown in Figure 2-5 (Emamipour et al., 2007b). Two annular cartridges of ACFC (American Kynol, ACC-5092-20) with a total weight of 73.5 g (for demonstration and proof of concepts, however the vessel can hold up to 180 g of ACFC) were located vertically in the cylindrical portion of the vessel. The external diameter of the cartridges was 3.1 cm with a length of 20 cm. Cartridge temperature is reported as the mean value for the two cartridges. During the adsorption cycle, the gas stream entered the bottom of the vessel’s cylindrical section, passed through the cartridges in parallel from the outside to the inside of the cartridges, and then exited through the top of the vessel. The organic vapor concentration was detected at the vessel’s outlet with a PID* (RAE Systems Inc., PDM-10A). Regeneration of the ACFC occurred by direct electrothermal heating of the adsorbent while air passed from the top of the vessel, through both cartridges from their inside to their outside, and then exited through the bottom of the vessel.

Figure 2-5. Bench-Scale ESA-SST System
2.2. Experimental Methodology

2.2.1. Calibration

The syringe pump injected liquid VOC (e.g., methyl ethyl ketone (MEK), HPLC grade, > 99% purity, Sigma Aldrich) into the dry and clean air stream to generate the vapor laden gas stream that contained the specified concentration of VOC. The calibration equations (concentration as a function of output signal) for the PID* and FID were obtained by running tests with known concentrations of the VOCs and recording the output signals from each of the VOC detectors.

2.2.2. ESA-VaPRRS

Experimental tests were completed in two phases: Screening experiments and Central Composite Designs (CCD) experiments (Kaldate, 2005). The purpose of the screening experiments was to identify the significant factors and their interactions. These factors were then tested with more resolution during the CCD experiments to determine the optimum operating conditions (Kaldate et al., 2003b; Emamipour et al., 2005). There were 20 screening experiments based on the Resolution IV 2^8-4 fraction (Kaldate, 2005), and 20 tests were completed for the CCD experiments. MEK was the adsorbate because it is one of the widely used solvents in the painting industry and it is often in dilute streams which is difficult to control. ACFC-5092-15 and ACFC-5092-20 adsorbents were tested during the screening experiments based on their cost and adsorption properties. A maximum adsorbent packing density of 55.1 kg/m³ was used because it was a physical limitation of the vessels. The lower packing density was determined by putting a constraint on the number of layers of cloth for each cartridge (6 layers) due to a concern about premature breakthrough of the adsorbate for a thinner layer of adsorbent. Temperature levels were selected to be higher than the boiling point of MEK (80°C) and less than melting point of Teflon (327°C). All adsorption tests were performed at an inlet air flow rate of 100 slpm. Nominal laboratory conditions were 25°C and 98 kPa. Vessels must be non-reactive to MEK and they also need to have different thermal conductivities to ensure that heat transfer effects of the vessels are included in the experiments. Aluminum and stainless steel 316 were good choices for this purpose. Experimental
factors and their low and high levels are summarized in Tables 2-1 and 2-2.

Table 2-1. Factors and Their Levels during the Screening Experiments

<table>
<thead>
<tr>
<th>Factor</th>
<th>Low Level</th>
<th>High Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of Adsorbent</td>
<td>ACFC-5092-15</td>
<td>ACFC-5092-20</td>
</tr>
<tr>
<td>Relative Pressure</td>
<td>0.002</td>
<td>0.01</td>
</tr>
<tr>
<td>ACFC Packing Density</td>
<td>18.3 kg/m³</td>
<td>55.1 kg/m³</td>
</tr>
<tr>
<td>Nitrogen Flow</td>
<td>0.005 slpm</td>
<td>1.0 slpm</td>
</tr>
<tr>
<td>Heating Algorithm</td>
<td>Constant Current</td>
<td>Constant Power</td>
</tr>
<tr>
<td>Vessel Material</td>
<td>Stainless steel</td>
<td>Aluminum</td>
</tr>
<tr>
<td>Number of Cartridges</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>Maximum Temperature</td>
<td>200°C</td>
<td>300°C</td>
</tr>
</tbody>
</table>

Table 2-2. Factors and Their Levels during the CCD Experiments

<table>
<thead>
<tr>
<th>Factor</th>
<th>Low Level</th>
<th>High Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative Pressure</td>
<td>0.00212</td>
<td>0.00677</td>
</tr>
<tr>
<td>ACFC Packing Density</td>
<td>23.5 kg/m³</td>
<td>47.0 kg/m³</td>
</tr>
<tr>
<td>Maximum Temperature</td>
<td>240°C</td>
<td>290°C</td>
</tr>
</tbody>
</table>

2.2.3. ESA-SST

All adsorption tests were performed at an inlet air flow rate of 100 slpm and 500 ppmv of MEK. As previously mentioned, nominal laboratory conditions were 25°C and 98 kPa. The gas stream initially by-passed the vessel before each adsorption test, until the MEK concentration in the air stream achieved its specified steady-state value. The adsorption cycle continued with the MEK laden gas stream passing through the vessel until the vessel’s adsorbent was > 98% saturated with MEK.

SST desorption tests were performed at an air flow rate of 20 slpm for the 500 ppmv
MEK test and 10 slpm for the 5,000 ppmv MEK test. The dynamic-tracking desorption test occurred with variable pre-defined outlet concentration set-points ranging from 250 ppmv to 5,000 ppmv, and an air flow rate of 10 slpm or 20 slpm. Multi-point calibrations were done at the gas flow rates used to complete the ESA-SST tests. The outlet gas stream was diluted with dry/clean air during the desorption cycles at high concentration (i.e., 5,000 ppmv) and the dynamic tracking test to prevent saturation of the PID* sensor.

The concentration of MEK at the vessel’s outlet during the regeneration tests was controlled by manipulating the electrical power applied to the ACFC, with the use of proportional-integral-derivative (PID) control, to achieve the desired set-point concentrations. The total mass of MEK that desorbed during each desorption cycle ($m_d$) was calculated using a material balance for the MEK:

$$m_d = \frac{Q_{reg} P^o M_{MEK}}{RT^o} \sum_{t=t_0}^{t_{reg}} \frac{y_{out}}{1 - y_{out}} \delta t$$

Eq 2-1

The extent of adsorbent regeneration ($\eta_{reg}$) is defined as the percent of the initially adsorbed MEK that was desorbed during the regeneration cycle:

$$\eta_{reg} = \frac{m_{d, reg}}{m_{ai}} \times 100$$

Eq 2-2

The extent of adsorbent regeneration was also characterized by assuming equilibrium conditions, $\eta_{reg, eq}$, and is defined as the percent of the adsorbed MEK that is desorbed during the regeneration cycle assuming the MEK in the gas stream is in equilibrium with adsorbed MEK:

$$\eta_{reg, eq} = \frac{m_{ai, eq} - m_{a, eq}}{m_{ai, eq}} \times 100$$

Eq 2-3

Equilibrium loadings were calculated based on the MEK concentrations in the bulk gas stream, temperature of the cartridge, and the Dubinin-Radushkevich (DR) isotherm equation.
2.3. Fluid flow and Heat Transfer Simulation

Modeling of gas flow and pressure drop (ΔP) patterns through the adsorption vessel and cartridges was initiated with the use of Computational Fluid Dynamics (CFD). CFD provides detailed 3-D quantitative descriptions of ΔP and gas flow patterns that cannot be easily measured with physical experiments. CFD solves flow equations numerically over small control volumes. The accuracy of the solution is influenced by the type and number of control volumes created. However, the simulations were repeated with different total number of control volumes until the results were reproducible.

The Reynolds Stress model was used in the computations. The 3-D Reynolds-averaged continuity and Navier–Stokes equations are given as:

\[
\frac{\partial (\rho u_i)}{\partial x_i} = 0 \quad \text{Eq 2-4}
\]

\[
\frac{\partial}{\partial x_j} \left( \rho u_i u_j \right) = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \right] + \frac{\partial}{\partial x_j} \left( \rho \bar{u}_i' \bar{u}_j' \right) \quad \text{Eq 2-5}
\]

Variables are described in the nomenclature section. The Reynolds stresses transport equation and the description of each term is as follows:

\[
\frac{\partial}{\partial x_k} \left( \rho u_k u_i' u_j' \right) = -\frac{\partial}{\partial x_k} \left( \rho u_j' u_i' u_k \right) + p \frac{\partial u_i'}{\partial x_j} + \delta_{ik} u_j' \frac{\partial u_i'}{\partial x_j} \frac{\partial u_k}{\partial x_k} \left[ \mu \frac{\partial}{\partial x_k} \left( \rho \bar{u}_j' \right) \right] \quad \text{Eq 2-6}
\]

\[
\begin{align*}
\text{Convection:} & \quad -\frac{\partial}{\partial x_k} \left( \rho u_j' u_k u_i' \right) \\
\text{Turbulent Diffusion:} & \quad p \frac{\partial u_i'}{\partial x_j} + \delta_{ik} u_j' \frac{\partial u_i'}{\partial x_j} \frac{\partial u_k}{\partial x_k} \\
\text{Molecular Diffusion:} & \quad \frac{\partial}{\partial x_k} \left[ \mu \frac{\partial}{\partial x_k} \left( \rho \bar{u}_j' \right) \right] \\
\text{Stress Production:} & \quad -p \left( u_j' \frac{\partial u_i'}{\partial x_k} + u_k' \frac{\partial u_i'}{\partial x_j} \right) \\
\text{PressureStrain:} & \quad p \left( \frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right) \\
\text{Dissipation:} & \quad -2\mu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k}
\end{align*}
\]

The gas stream flowing through the annular cartridges is modeled as if the cartridges are porous monoliths. The porous media is modeled by the addition of a momentum source term to the fluid flow equations. However permeability and inertial resistance
factors of the porous media are needed in the momentum source term and they are obtained experimentally as described in the next section. Theoretical-experimental models are used for turbulent diffusion, pressure strain, and dissipation to provide a sufficient number of equations to simulate the gas flow pattern while obtaining numerical closure. Details about the models that approximate these parameters are described in the FLUENT manual.

GAMBIT, which is FLUENT’s preprocessor was used to develop the geometry and meshes for the calculations. Solid parts of the adsorption vessel and plumbing were treated as impervious volumes for fluid flow in the computational domain. The cartridges were meshed using the map scheme. The Cooper Tool was then used to mesh the adsorption vessel. The z direction was chosen as the main direction for the meshing. Finally, the velocity of the gas at the vessel’s inlet and the total pressure of the gas at the vessel’s outlet were chosen as the boundary conditions.

The 3-D continuity, Navier–Stokes, and Reynolds-stresses transport equations were then solved using Fluent 6. Computational mesh was generated by using Gambit and results were visualized using TecPlot™ (Figure 2-6. Simulation Flowchart of Fluid Flow and Pressure Drop). The standard scheme specified in FLUENT was used to interpolate pressure values and the second order upwind scheme was applied to all other variables, because the model provided stable results with these schemes.

The pressure gradient through the cartridge is expressed as:

$$\nabla P = -\frac{\mu}{\alpha} v - C \left( \frac{1}{2} \rho v |v| \right)$$

Eq 2-7

Where $\alpha$ is the permeability and C is the inertial resistance factor (the extra resistance caused by the porous medium to fluid flow, caused by local accelerations within the tortuous pore volume).
Integration of Eq 2-7 while neglecting tangential and axial components provides the following analytical expression for pressure drop in the radial direction across the

\[ \Delta P = \zeta_i - P_o = \frac{\mu}{\alpha} \frac{Q}{2\pi L} \ln \left( \frac{r_o}{r_i} \right) + \frac{\rho C Q^2}{8\pi^2 L^2} \left( \frac{1}{r_i} - \frac{1}{r_o} \right) \]  

Eq 2-8

Values of \( \alpha \) and \( C \) were then obtained by curve fitting experimental \( \Delta P \) data for each cartridge of ACFC with Eq 2-8.

CFD simulation of unsteady-state heating of the cartridges in the vessel is performed by solving fluid flow and heat transfer equations using FLUENT. Details of equations are available in the FLUENT 6 User’s Guide (2001).

2.4. Simulation of Heat and Mass Transfer in ESA

Schematic of absorption vessel containing ACFC cartridges is demonstrated in Figure 2-7. The model consists of: a) mass balances for organic vapors in the adsorption vessel
Figure 2-7. Schematic of Absorption Vessel Containing Two ACFC Cartridges

and b) energy balances for the adsorbent, carrier gas, vapor, and fittings. All equations are developed for two cylindrical cartridges in the vessel, but they can be extended for different configurations of the cartridges. The assumptions of models are:

- Cartridges are cylindrical.
- Gas velocity is only changing in the radial direction.
- Temperature is only changing in the radial direction.
- Heat transfer through the top plate of the vessel is negligible.
- Ideal gas law is applicable.
- There is no gas flow through the top and bottom of cartridges where is connected to solid tubes and plugs.
2.4.1. Mass Balance for Adsorbate in the Cartridges

Differential equation of a specie balance can be obtained by applying a mass balance on the organic vapor flowing in and out of a tiny control volume in the cartridges. There is no fluid flow in the top and bottom of cartridges where are connected to tubes or plugs. These parts of cartridges are referred to as “mounted section”, and the rest as “non-mounted section”. The height of each control volumes is equal to the height of that section of cartridges. The differential equation is formed by taking the thickness of each control volume, \( \delta r \), to approach its zero limit (Emamipour et al., 2007a & 2008b).

2.4.1.1. Non-Mounted Section

Gas phase:

The differential equation of a specie balance in the gas phase can be expressed as:

\[
\frac{\partial C_A}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r v r C_A \right) + k_m a \left( C^v_A - C_A \right)
\]

The left term is accumulation, the first term at the right is advection, and the second term at the right is convection. By assuming constant mass flow of inert gas (e.g., air), superficial gas velocity can be expressed as:
$$v_r = Q^* \frac{T_g}{T^*} \frac{P^*}{P} \frac{1}{4\pi R L}$$ \hspace{1cm} \text{Eq 2-10}$$

$C^*_A$ is equilibrium concentration of the organic vapor at the interface of the gas and adsorbent fibers, which can be related to the concentration of organic vapor in the fibers by using an adsorption isotherm equation such as Direct Quantitative Structure-Activity Relationship (DQSAR) (Ramirez, 2005):

$$C_A^* = \frac{P^*}{R_g T_s \exp \left( \frac{1}{R_g T_s} \left< \frac{\ln \left( \frac{q M_A}{\rho_{l_A} w_o} \right)}{\kappa} \right> \right)} \hspace{1cm} \text{Eq 2-11}$$

The boundary and initial conditions for the Eq 2-9 are:

\begin{align*}
  r &= r_i \quad C_A = C_{A,in} \\
  t &= 0 \quad C_A = C^i_A
\end{align*}

Solid phase:

Although diffusion takes place inside the fibers (Lordgooei, 1999, Lordgooei et al., 2001), LDF (Linear Driving Force) method was used to approximate the mass transfer for the solid phase (Yang, 1999; Petkovska et al., 2005; Petkovska et al., 2007; Yu et al., 2007) in order to reduce the computational time and avoid the numerical instability. The differential equation of species balance in the fibers can be expressed as:

$$\rho_b \frac{\partial q}{\partial t} = k_m a \left( C_A - C_A^* \right) \hspace{1cm} \text{Eq 2-12}$$

The left term describes accumulation and the right term describes convection mass transfer. The initial condition is:

\begin{align*}
  t &= 0 \quad q = q^i
\end{align*}

2.4.1.2. Mounted Section

There is no fluid flow in this section of the cartridge. Mass transfer in this part occurs
by diffusion.

Gas phase:

By replacing advection term in Eq 2-9 with the diffusion term and the following differential equation is obtained:

$$\varepsilon \frac{\partial C_A}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r D_{AB}^{\text{eff}} \frac{\partial C_A}{\partial r} \right) + k_m a C_A^{\text{r}} - C_A^{\text{t}}$$

Eq 2-13

Boundary and initial conditions are:

$$r = r_i \quad \frac{\partial C_A}{\partial r} = 0$$

$$r = r_o \quad -D_{AB}^{\text{eff}} \frac{\partial C_A}{\partial r} = k_m a C_A^{\text{r}} - C_A^{\text{b}_2}$$

$$t = 0 \quad C_A = C_A^{i}$$

Solid phase:

The same differential equation that was obtained for the non-mounted section can be used here:
\[ \rho_b \frac{\partial q}{\partial t} = k_m a \sum A - C^\gamma \]  

\[ t = 0 \quad q = q^i \]

2.4.2. Energy Balance for the Cartridges

2.4.2.1. Non-Mounted Section

Gas phase:

The differential equation of energy balance in the gas phase can be expressed as:

\[ \varepsilon \rho g c_{pe} \frac{\partial T_g}{\partial t} = \frac{1}{r} \left( r k_{eff} \frac{\partial T_g}{\partial r} \right) - \rho g c_{pe} v r \frac{\partial T_g}{\partial r} + h_b a \left( F_s - T_g \right) \]  

\[ \text{Eq 2-15} \]

The left term is accumulation, the first term at the right is conduction, the second term is advection, and the last term is convection. The boundary and initial conditions are:
Solid phase:

Energy balance for the fibers can be expressed as:

\[
\frac{\partial}{\partial t} \left( \rho_b c_{p,b} \right) + \frac{\partial}{\partial r} \left( \rho_b c_{p,b} v \right) = -k_{eff} \frac{\partial T_c}{\partial r} + \frac{\partial}{\partial r} \left( \rho_b c_{p,b} \right) \frac{\partial T_c}{\partial r} - \rho_b A H_{ads} \frac{\partial q}{\partial t} - h_{b,a} \frac{\partial T_c}{\partial r} - T_c - T_g
\]

The left term describes accumulation of heat, the first term to the right of the equal sign is heat conduction, the second term is heat generation, the third term is heat of adsorption, and the last term is heat convection. The boundary and initial conditions are:

\[
r = r_i \quad -k_{eff} \frac{\partial T_c}{\partial r} = h_1 \varepsilon \frac{\partial T_b}{\partial r} - T_c
\]
\[
r = r_o \quad -k_{eff} \frac{\partial T_c}{\partial r} = h_2 \varepsilon \frac{\partial T_b}{\partial r} - T_{b2}
\]
\[
t = 0 \quad T_c = T_c^i
\]

2.4.2.2. Mounted Section

There is no fluid flow in this section of the cartridge. Heat transfer in this part occurs by conduction.

Gas phase:

By removing advection term from Eq 2-15 the following differential equation is obtained:
\[ \varepsilon \rho_c c_{p,g} \frac{\partial T_g}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r k_{g e, eff} \frac{\partial T_g}{\partial r} \right) + h_{b,a} \left( \mathbf{e}_g - T_g \right) \sim \]  

Eq 2-17

The boundary and initial conditions are:

\[
\begin{align*}
\begin{cases}
   k_{g e, eff} \frac{\partial T_g}{\partial r} = \varepsilon k_{n1} \frac{\partial T_{n1}}{\partial r} & \text{top} \\
   k_{g e, bottom} L_{c,btm} \frac{\partial T_g}{\partial r} = \varepsilon \int_{L_{c,btm}} k_{plg} \frac{\partial T_{plg}}{\partial r} \, dz & \text{bottom}
\end{cases}
\end{align*}
\]

\[ r = r_i \quad -k_{g e} \frac{\partial T_g}{\partial r} = h_2 \varepsilon \left( T_g - T_{bg} \right) \sim \]

\[ r = r_o \]

\[ t = 0 \quad T_g = T_{g}^i \]

Solid phase:

The same differential equation that was obtained for the non-mounted section is also used here:

\[ \Phi_b c_{p,s} + \rho_b q M_A c_{p,l} \frac{\partial T_c}{\partial t} = \]

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r k_{c e, eff} \frac{\partial T_c}{\partial r} \right) + \dot{q} - \rho_b \Delta H_{ads} \frac{\partial \dot{q}}{\partial t} - h_{b,a} \left( \mathbf{e}_c - T_g \right) \sim \]  

Eq 2-18
Boundary and initial conditions are:

\[
\begin{align*}
\text{top} & \quad r = r_i \\
\text{bottom} & \quad r = r_o \\
& \quad -k_c^{\text{eff}} \frac{\partial T_c}{\partial r} = \epsilon \left( \frac{\partial}{\partial r} \right)_{r_i} \frac{\partial T_{k1}}{\partial r} \\
& \quad -k_g^{\text{eff}} \frac{\partial T_g}{\partial r} = \epsilon \left( \frac{\partial}{\partial r} \right)_{r_o} \frac{\partial T_{p_{l,b}}}{\partial r} \\
\end{align*}
\]

\[t = 0 \quad T_g = T_{g_i}\]

2.4.3. Energy Balance for Vessel Wall

The differential equation of energy balance can be obtained by equaling the accumulation and conduction terms:

\[
\rho_w c_{p,w} \frac{\partial T_w}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r k_w \frac{\partial T_w}{\partial r} \right)
\]

Eq 2-19

With following boundary and initial conditions:

\[
\begin{align*}
\text{top} & \quad r = r_i \\
& \quad -k_w \frac{\partial T_w}{\partial r} = h_3 \epsilon \left( \frac{\partial}{\partial r} \right)_{r_i} T_{w-h} \\
\text{bottom} & \quad r = r_o \\
& \quad -k_w \frac{\partial T_w}{\partial r} = h_4 \epsilon \left( \frac{\partial}{\partial r} \right)_{r_o} T_{amb-h} \\
\end{align*}
\]

\[t = 0 \quad T_w = T_{w_i}\]

2.4.4. Energy Balance for the Bulk Gas

2.4.4.1. Inlet Tube

Differential equation for the temperature of gas in the inlet tubes can be expressed as:

\[
\rho_g V_{b_l} c_{p,g} \frac{\partial T_{b_l}}{\partial t} = -p^\omega \int_{T_{g_i}}^{T_{g_f}} c_{p,g} dT_g + h_i A_{cl} \left( \epsilon \left( \frac{\partial}{\partial r} \right)_{r_i} T_{g-h} \right)_{r_i} - T_{b_{l-h}} + h_i A_{cl} \epsilon \left( \frac{\partial}{\partial r} \right)_{r_i} T_{g-h} - T_{b_{l-h}}
\]

Eq 2-20

The left term describes accumulation, the integral term at the right describes
advection, and the other terms describe convection. This equation requires one initial condition:

\[ t = 0 \quad T_{b1} = T_{b1}^i \]

2.4.4.2. Adsorption Vessel

Differential equation is similar to the one for the inlet tubes except that convective heat transfer from the vessel’s wall is added:

\[
\rho_g V_{b2} C_{p,g} \frac{\partial T_{b2}}{\partial t} = -\rho^o Q^o \left[ c_{p,g} \frac{\partial T_g}{\partial t} + h_2 A_c e_c \left( \frac{\partial T}{\partial r} \right) \right]_{r=ro} - T_{b2}^i
\]

Eq 2-21

\[
h_2 A_c e_g \left( \frac{\partial T}{\partial r} \right)_{r=ro} - T_{b2}^i + h_3 A_w \left( T_w - T_{b2}^i \right)
\]

The initial condition is:

\[ t = 0 \quad T_{b2} = T_{b2}^i \]

2.4.5. Energy Balance for the Inlet Tubes

Inlet tubes may be divided in two parts. Part (1) is touching the cartridges, part (2) is not in direct contact with the cartridges.

1. Assuming heat transfer occurs mainly in the \( r \) direction, the differential equation for the temperature can be expressed as:

\[
\rho_{\text{u}} c_{\text{p,\text{u}}} \frac{\partial T_{\text{g1}}}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r k_{\text{u}} \frac{\partial T_{\text{g1}}}{\partial r} \right)
\]

Eq 2-22

2. This part can be considered as a fin. The differential equation for temperature is:
\[ \rho_{w} c_{w} A \frac{\partial T_{w}}{\partial t} = A \frac{\partial}{\partial z} \left( k \frac{\partial T_{w}}{\partial z} \right) - h_{in} \phi_{in} \left( T_{w} - T_{b1} \right) - h_{out} \phi_{out} \left( T_{w} - T_{b2} \right) \quad \text{Eq 2-23} \]

\( h_{in} \) and \( h_{out} \) are convective heat transfer coefficients inside the tubes and outside the tubes respectively. \( h_{out} \) is assumed to be zero where tubes are touching the Teflon top plate.

The boundary and initial conditions are:

\[
\begin{align*}
  r &= r_1, \quad -k \frac{\partial T_{w1}}{\partial r} = h_{1} \phi_{b1} - T_{w1} \\
  r &= r_0, \quad T_{w1} = T_{c} \\
  z &= L_{w1}, \quad T_{w1} = T_{w2} \\
  z &= L_{w2}, \quad \left\{ \begin{array}{l} T_{w2} = T_{w3} \\ k \frac{\partial T_{w2}}{\partial z} = k \frac{\partial T_{w3}}{\partial z} \end{array} \right. \\
  z &= L_{w3}, \quad \left\{ \begin{array}{l} T_{w3} = T_{w4} \\ k \frac{\partial T_{w3}}{\partial z} = k \frac{\partial T_{w4}}{\partial z} \end{array} \right. \\
  z &= L_{w4}, \quad T_{w4} = T_{amb} \\
  t &= 0, \quad T_{n1} = T_{n1}^i; \quad T_{n2} = T_{n2}^i; \quad T_{n3} = T_{n3}^i; \quad T_{n4} = T_{n4}^i
\]

2.4.6. Energy Balance for the Plugs

The aspect ratio of the plugs is 0.75. The two dimensional differential equation for the plug’s temperature can be expressed as:

\[ \rho_{plg} c_{plg} \frac{\partial T_{plg}}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r k_{plg} \frac{\partial T_{plg}}{\partial r} \right) + \frac{\partial}{\partial z} \left( k_{plg} \frac{\partial T_{plg}}{\partial z} \right) \quad \text{Eq 2-24} \]

with the following boundary and initial conditions:

\[ r = 0, \quad \frac{\partial T_{plg}}{\partial r} = 0 \]
\[ r = r_{plg} \begin{cases} T_{plg} = T_c & \text{top} \\ -k_{plg} \frac{\partial T_{plg}}{\partial r} = h_5 \left( \phi_{plg} - T_{b2} \right) & \text{bottom} \end{cases} \]

\[ z = 0 \quad -k_{plg} \frac{\partial T_{plg}}{\partial z} = h_6 \left( \phi_{b2} - T_{plg} \right) \]

\[ z = l_{plg} \quad -k_{plg} \frac{\partial T_{plg}}{\partial z} = h_7 \left( \phi_{plg} - T_{b1} \right) \]

\[ t = 0 \quad T_{plg} = T_{plg}^i \]

2.4.7. Numerical Methodology

The partial differential equations were converted to algebraic equations by using finite volume method in space and Crank-Nicholson method in time. The resulting set of algebraic equations were then solved by using the Gauss-Seidel method to calculate the adsorbate concentration profiles in the gas and solid phases, as well as temperature profiles of gas and solid phases. Since amount of power applied to the adsorbent is unknown in each time step for steady-state tracking desorption, a trial and error was used to calculate the heat generation term in each time interval. For VaPRRS amount of liquid recovered was calculated by assuming that outlet gas is saturated with the organic vapor. Programming was performed in C++ version 5.

The average absolute errors (AAEs) will be used to compare the difference between modeled and experimental values, and is defined by:

\[
\text{AAE} = \frac{1}{N} \sum_{j=1}^{N} \left[ \frac{|x_{i,M} - x_{i,E}|}{x_{i,E}} \times 100 \right]
\]

where \( N \) is the total number of corresponding data points, and \( x_{i,M} \) and \( x_{i,E} \) represent corresponding modeled and experimental values of properties of interest.
3. RESULTS AND DISCUSSION

3.1. Experimental Results

3.1.1. ESA-VaPRRS

3.1.1.1. Screening Experimental Tests

The purpose of the screening experiments is to provide input data for the analytical methods developed by Kaldate (2005). The experimental results presented here were used by Kaldate (2005) to identify the design parameters that are important in terms of energy consumption per unit mass of liquid recovered. The experimental conditions for the screening experiments are shown in Table 3-1. The main response of interest for the experiments is the energy/mass of MEK recovered as a liquid. However, other parameters that are recorded during the experiments are: a) percentage liquid recovery, b) organic vapor concentration at the inlet and outlet of the adsorbers, and in recycle loop, c) gas flow rate at inlet, outlet and in the recycle loop, d) nitrogen flow, e) temperature at inlet, outlet, condensate and recycle loop, f) current, g) voltage, h) resistance of cartridges, i) temperature of cartridges, temperature of vessel wall, j) adsorption capacity and k) pressure drop across each adsorber. Vessel 1 and vessel 2 are made of aluminum and stainless steel, respectively, to be able to evaluate which material should be used to build prototype vessels (Kaldate, 2005).

Examples of experimental results for run no. 3 of the screening tests with conditions specified in Table 3-2 are provided in Figure 3-1 through Figure 3-8. These results describe MEK concentration at the outlet of the system (Figure 3-1), MEK concentration in the recycle gas stream (Figure 3-2), cartridge temperatures (Figure 3-3 and Figure 3-4), wall temperatures (Figure 3-5), recycle gas stream temperature (Figure 3-6), and electrical power and current (Figure 3-7 and Figure 3-8) as a function of time for two hours of continuous operation.
Table 3-1. Screening Experiments Design

<table>
<thead>
<tr>
<th>Run no.</th>
<th>Adsorbent</th>
<th>Relative Pressure</th>
<th>Packing Density (g/l)</th>
<th>Nitrogen Flow (slpm)</th>
<th>Maximum Heating Temperature (°C)</th>
<th>Number of Cartridges</th>
<th>Heating Algorithm (Constant parameter)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ACFC-20</td>
<td>0.00169</td>
<td>18.3</td>
<td>1</td>
<td>300</td>
<td>2</td>
<td>Current</td>
</tr>
<tr>
<td>2</td>
<td>ACFC-15</td>
<td>0.00423</td>
<td>36.7</td>
<td>0.5025</td>
<td>250</td>
<td>2</td>
<td>Current</td>
</tr>
<tr>
<td>3</td>
<td>ACFC-15</td>
<td>0.00677</td>
<td>55.1</td>
<td>1</td>
<td>300</td>
<td>2</td>
<td>Current</td>
</tr>
<tr>
<td>4</td>
<td>ACFC-15</td>
<td>0.00423</td>
<td>36.7</td>
<td>0.5025</td>
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<td>Power</td>
</tr>
<tr>
<td>5</td>
<td>ACFC-15</td>
<td>0.00677</td>
<td>18.3</td>
<td>0.005</td>
<td>300</td>
<td>2</td>
<td>Power</td>
</tr>
<tr>
<td>6</td>
<td>ACFC-20</td>
<td>0.00677</td>
<td>55.1</td>
<td>1</td>
<td>300</td>
<td>4</td>
<td>Power</td>
</tr>
<tr>
<td>7</td>
<td>ACFC-15</td>
<td>0.00169</td>
<td>55.1</td>
<td>0.005</td>
<td>300</td>
<td>4</td>
<td>Current</td>
</tr>
<tr>
<td>8</td>
<td>ACFC-20</td>
<td>0.00677</td>
<td>18.3</td>
<td>1</td>
<td>200</td>
<td>2</td>
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</tr>
<tr>
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<td>1</td>
<td>200</td>
<td>4</td>
<td>Current</td>
</tr>
<tr>
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<td>18.3</td>
<td>0.005</td>
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<td>Current</td>
</tr>
<tr>
<td>11</td>
<td>ACFC-20</td>
<td>0.00169</td>
<td>55.1</td>
<td>0.005</td>
<td>300</td>
<td>2</td>
<td>Power</td>
</tr>
<tr>
<td>12</td>
<td>ACFC-15</td>
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<td>2</td>
<td>Power</td>
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<tr>
<td>13</td>
<td>ACFC-15</td>
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<td>0.5025</td>
<td>250</td>
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<td>Power</td>
</tr>
<tr>
<td>14</td>
<td>ACFC-15</td>
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<td>55.1</td>
<td>0.005</td>
<td>200</td>
<td>4</td>
<td>Power</td>
</tr>
<tr>
<td>15</td>
<td>ACFC-20</td>
<td>0.00677</td>
<td>55.1</td>
<td>0.005</td>
<td>200</td>
<td>2</td>
<td>Current</td>
</tr>
<tr>
<td>16</td>
<td>ACFC-15</td>
<td>0.00423</td>
<td>36.7</td>
<td>0.5025</td>
<td>250</td>
<td>2</td>
<td>Current</td>
</tr>
<tr>
<td>17</td>
<td>ACFC-20</td>
<td>0.00169</td>
<td>18.3</td>
<td>0.005</td>
<td>200</td>
<td>4</td>
<td>Power</td>
</tr>
<tr>
<td>18</td>
<td>ACFC-15</td>
<td>0.00169</td>
<td>18.3</td>
<td>1</td>
<td>300</td>
<td>4</td>
<td>Power</td>
</tr>
<tr>
<td>19</td>
<td>ACFC-20</td>
<td>0.00677</td>
<td>18.3</td>
<td>0.005</td>
<td>300</td>
<td>4</td>
<td>Current</td>
</tr>
<tr>
<td>20</td>
<td>ACFC-15</td>
<td>0.00677</td>
<td>18.3</td>
<td>1</td>
<td>200</td>
<td>4</td>
<td>Current</td>
</tr>
</tbody>
</table>
Table 3-2. Level of Factors for Run No. 3 of the Screening Tests

<table>
<thead>
<tr>
<th>Factor</th>
<th>Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of Adsorbent</td>
<td>ACFC-5092-15</td>
</tr>
<tr>
<td>Relative Pressure</td>
<td>0.00677</td>
</tr>
<tr>
<td>Packing Density</td>
<td>55.1 kg/m³</td>
</tr>
<tr>
<td>Nitrogen Flow</td>
<td>1.0 slpm</td>
</tr>
<tr>
<td>Heating Algorithm</td>
<td>Constant Current</td>
</tr>
<tr>
<td>Number of Cartridges</td>
<td>2</td>
</tr>
<tr>
<td>Maximum Temperature</td>
<td>300°C</td>
</tr>
</tbody>
</table>

Concentration of MEK in the outlet gas stream is less than 1 ppmv until the occurrence of breakthrough, where the concentration starts to increase until 5% of inlet concentration (i.e., 5% of 800 ppmv, Figure 3-1). The concentration of MEK then decreases abruptly when the inlet gas stream is switched to the stand-by vessel and the saturated adsorbent is regenerated. Sudden increases and subsequent decreases in MEK concentration within the recycle stream, as described in Figure 3-2, are caused by the recycling of the concentrated vapor from the condensate reservoir that is located downstream of the vessel and is experiencing a regeneration cycle. Temperatures of the cartridges during regeneration increase quickly (less than 6 min) to 300°C and then decrease exponentially. The change of slope at 80°C during the cooling period is caused by switching off the nitrogen flow through the cartridges (Figure 3-3 and Figure 3-4). Such response is due to advection heat transfer by nitrogen flow increasing the heat transfer from the ACFC’s fibers. Temperatures of the cartridges are very close for each vessel (average standard deviation = 2.0°C and 4.4°C for aluminum and stainless steel vessels, respectively) indicating similarity of the cartridges for each vessel type. Maximum temperature of the vessel wall is slightly (less than 3°C) more for the aluminum vessel when compared to the stainless steel vessel (Figure 3-5). This was expected, because aluminum has faster heat transfer properties than stainless steel. However, the temperature of the recycle gas stream during the regeneration cycles were
very similar for the aluminum and stainless steel vessels, because the temperature of the
gas stream was measured sufficiently downstream of the vessel to allow the low flow rate
recycle stream to cool to similar temperatures (Figure 3-6).

Figure 3-1. Inlet and Outlet Concentration of MEK during an Adsorption Cycle as a
Function of Time for Run No. 3 of the Screening Tests

Figure 3-2. Concentration of MEK in the Recycle Gas Stream as a Function of Time for
Run No. 3 of the Screening Tests
Figure 3-3. Temperature of the ACFC Cartridges in the Aluminum Vessel as a Function of Time for Run No. 3 of the Screening Tests; T101-T104 indicate thermocouple numbers measuring the temperature of the cartridges in vessel 1

Figure 3-4. Temperature of ACFC Cartridges in the Stainless Steel Vessel as a Function of Time for Run No. 3 of the Screening Tests; T201-T204 indicates thermocouple numbers measuring the temperature of the cartridges in vessel 1
Figure 3-5. Wall Temperatures as a Function of Time for Run No. 3 of the Screening Tests; T105 and T205 indicate thermocouples connected to vessel 1 and vessel 2, respectively.

Figure 3-6. Recycle Gas Stream Temperature as a Function of Time for Run No. 3 of the Screening Tests. T106 and T206 indicate thermocouples connected to the outlets of vessel 1 and vessel 2, respectively.
The changes in electrical power and current during the desorption cycles are extremely rapid and they appear as step functions (Figure 3-7). However, expansion of
one of the power and current applications during a regeneration cycle indicates a rapid increase, exponential decay, and then a rapid decrease in power, with a more typical step function for the current (Figure 3-8). Exponential decay in power, while current is constant, indicates reduction of cartridge resistance during heating. This is because resistivity of ACFC is temperature dependent and decreases with increasing temperature over the measured temperature range.

The energy consumption/mass of liquid recovered can be calculated by integrating the power over time and dividing by mass of liquid recovered. The final results for screening experiments are summarized in Table 3-3.

Table 3-3. Energy per Unit Mass of Liquid Recovered for Different Runs of Screening Experiments

<table>
<thead>
<tr>
<th>Run No.</th>
<th>Number of cycles</th>
<th>Energy/MEK recovered (J/g)</th>
<th>Run No.</th>
<th>Number of cycles</th>
<th>Energy/MEK recovered (J/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10</td>
<td>17,967</td>
<td>11</td>
<td>4</td>
<td>10,106</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>4,689</td>
<td>12</td>
<td>5</td>
<td>11,107</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>4,272</td>
<td>13</td>
<td>4</td>
<td>5,573</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>5,536</td>
<td>14</td>
<td>22</td>
<td>22,158</td>
</tr>
<tr>
<td>5</td>
<td>7</td>
<td>10,270</td>
<td>15</td>
<td>23</td>
<td>20,607</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>6,789</td>
<td>16</td>
<td>5</td>
<td>5,334</td>
</tr>
<tr>
<td>7</td>
<td>4</td>
<td>9,072</td>
<td>17</td>
<td>15</td>
<td>119,427</td>
</tr>
<tr>
<td>8</td>
<td>11</td>
<td>15,913</td>
<td>18</td>
<td>9</td>
<td>109,668</td>
</tr>
<tr>
<td>9</td>
<td>11</td>
<td>135,702</td>
<td>19</td>
<td>20</td>
<td>21,155</td>
</tr>
<tr>
<td>10</td>
<td>18</td>
<td>98,991</td>
<td>20</td>
<td>13</td>
<td>26,039</td>
</tr>
</tbody>
</table>

The experimental data from the screening experiments were fed to an optimization model developed by Kaldate (2005) and it was observed that “nitrogen flow” and “heating algorithm” are insignificant factors; in other words, the energy requirements for MEK liquid recovery do not depend on the levels of these factors in the range of values considered for the screening experiments. Therefore, these factors can be eliminated from the CCD experiments.
Though the purpose of the screening experiments is to determine the significant factors for further analysis and not to specify a model for the response, the final equation for response in terms of the “coded” factors helps in determining which levels of each of the significant factors are better for further studies. The low and high levels of the factors shown in Table 2.1 are coded as \(-1\) and \(+1\). For qualitative factors, this decision to set these levels leads advantageously to reducing the future experimental complexity. The model equation in terms of the coded factors was obtained by Kaldate (2005) and is shown below:

\[
\frac{1}{\sqrt{\text{Energy/mass recovered}}} = 7.57 \times 10^{-3} - 4.59 \times 10^{-4} \times A + 1.42 \times 10^{-3} \times B + 1.65 \times 10^{-3} \times C + 1.81 \times 10^{-3} \times E - 1.19 \times 10^{-3} \times F + 6.32 \times 10^{-4} \times G - 8.21 \times 10^{-4} \times A \times C + 9.18 \times 10^{-4} \times F \times G
\]

Where:

\(A\) = Type of adsorbent

\(B\) = Relative pressure

\(C\) = Packing density

\(E\) = Maximum heating temperature

\(F\) = Number of cartridges

\(G\) = Vessel material

ACFC-15 with stainless steel fittings and with a two cartridge configuration leads to lower energy/mass of liquid MEK recovered causing these factors to be fixed at these levels.

3.1.1.2. Central Composite Design Experimental Tests

The experimental conditions for the CCD experiments are shown in
Nitrogen flow was fixed at 1 slpm and constant current was chosen as heating algorithm.

Table 3-4. Central Composite Design

<table>
<thead>
<tr>
<th>Run no.</th>
<th>Relative Pressure (x10^{-3})</th>
<th>Maximum Heating Temperature (°C)</th>
<th>Packing Density (g/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.44^a</td>
<td>265</td>
<td>35.25</td>
</tr>
<tr>
<td>2</td>
<td>6.77</td>
<td>290</td>
<td>23.50</td>
</tr>
<tr>
<td>3</td>
<td>2.12</td>
<td>240</td>
<td>23.50</td>
</tr>
<tr>
<td>4</td>
<td>0.54</td>
<td>265</td>
<td>35.25</td>
</tr>
<tr>
<td>5</td>
<td>6.77</td>
<td>240</td>
<td>23.50</td>
</tr>
<tr>
<td>6</td>
<td>2.12</td>
<td>290</td>
<td>23.50</td>
</tr>
<tr>
<td>7</td>
<td>4.44</td>
<td>265</td>
<td>35.25</td>
</tr>
<tr>
<td>8</td>
<td>6.77</td>
<td>290</td>
<td>47.00</td>
</tr>
<tr>
<td>9</td>
<td>4.44</td>
<td>222</td>
<td>35.25</td>
</tr>
<tr>
<td>10</td>
<td>4.44</td>
<td>265</td>
<td>35.25</td>
</tr>
<tr>
<td>11</td>
<td>4.44</td>
<td>265</td>
<td>35.25</td>
</tr>
<tr>
<td>12</td>
<td>4.44</td>
<td>307</td>
<td>35.25</td>
</tr>
<tr>
<td>13</td>
<td>4.44</td>
<td>265</td>
<td>55.01</td>
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<tr>
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<td>4.44</td>
<td>265</td>
<td>15.49</td>
</tr>
<tr>
<td>15</td>
<td>8.35</td>
<td>265</td>
<td>35.25</td>
</tr>
<tr>
<td>16</td>
<td>2.12</td>
<td>240</td>
<td>47.00</td>
</tr>
<tr>
<td>17</td>
<td>4.44</td>
<td>265</td>
<td>35.25</td>
</tr>
<tr>
<td>18</td>
<td>6.77</td>
<td>240</td>
<td>47.00</td>
</tr>
<tr>
<td>19</td>
<td>4.44</td>
<td>265</td>
<td>35.25</td>
</tr>
<tr>
<td>20</td>
<td>2.12</td>
<td>290</td>
<td>47.00</td>
</tr>
</tbody>
</table>

^a = 4.44\times10^{-3}$
The final results for all CCD experiments are summarized in Table 3-5. Results were used in the optimization model by Amit Kaldate and a new value of 4.7 W/g for amount of power applied per unit mass of ACFC was obtained. This is 33% reduction over the previous value of 7 W/g.

Table 3-5. Energy per Unit Mass of Liquid Recovered for Different Runs of CCD Experiments

<table>
<thead>
<tr>
<th>Run No.</th>
<th>Number of Cycles</th>
<th>Energy/MEK Recovered (J/g)</th>
<th>Run No.</th>
<th>Number of Cycles</th>
<th>Energy/MEK Recovered (J/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>5,344</td>
<td>11</td>
<td>4</td>
<td>5,191</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>6,775</td>
<td>12</td>
<td>5</td>
<td>5,416</td>
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<tr>
<td>3</td>
<td>5</td>
<td>13,756</td>
<td>13</td>
<td>4</td>
<td>3,088</td>
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<tr>
<td>4</td>
<td>4</td>
<td>6,905</td>
<td>14</td>
<td>22</td>
<td>24,463</td>
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<td>5</td>
<td>7</td>
<td>5,927</td>
<td>15</td>
<td>23</td>
<td>2,512</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>9,298</td>
<td>16</td>
<td>5</td>
<td>5,346</td>
</tr>
<tr>
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<td>4</td>
<td>4,039</td>
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<td>15</td>
<td>4,963</td>
</tr>
<tr>
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<td>11</td>
<td>4,589</td>
<td>18</td>
<td>9</td>
<td>4,200</td>
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<tr>
<td>9</td>
<td>11</td>
<td>4,838</td>
<td>19</td>
<td>20</td>
<td>4,548</td>
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<tr>
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<td>18</td>
<td>4,938</td>
<td>20</td>
<td>13</td>
<td>3,399</td>
</tr>
</tbody>
</table>

The model equations in terms of the coded and actual factors are shown below (Kaldate, 2005).

Final Equation in Terms of Coded Factors is:

\[
\text{Log}_{10}\left(\frac{\text{Energy/Mass Recovered}}{\text{MEK}}\right) = 3.68 - 0.13 \times A - 0.014 \times B - 0.27 \times C - 0.018 \times A^2 + 0.014 \times B^2 + 0.095 \times C^2 + 0.058 \times A \times B + 0.066 \times A \times C - 5.759 \times 10^{-3} \times B \times C + 0.12 \times A^2 \times C + 0.071 \times A \times C^2
\]

Final Equation in Terms of Actual Factors:

\[
\text{Log}_{10}\left(\frac{\text{Energy/Mass Recovered}}{\text{MEK}}\right) = 6.05 + 497.1 \times \text{Relative Pressure} - 0.016 \times \text{max Heating Temperature} + 0.030 \times \text{Packing Density} - 70684.05 \times \text{Relative Pressure}^2 + 2.22 \times 10^{-5} \times \text{max Heating Temperature}^2 - 2.92
\]
Based on analysis performed by Kaldate (2005), at lower relative pressures, higher heating temperature reduces energy requirements. However, at higher relative pressures, lower heating temperature would be slightly better in order to reduce the energy consumption. It was also found that higher packing density always leads to less energy consumption as compared to lower packing density, even though the difference between the energy requirements is reduced at higher relative pressures.

Reduction in the amount of power applied per unit mass of ACFC in the vessel is another important result of the CCD experiment. The new value of this energy requirement, 4.7 W/g ACFC represents a reduction of 32.8% over the current value of 7 W/g ACFC. It should be noted that, objective function for optimization is energy per unit mass of liquid MEK recovered. The new value of 4.7 W/g ACFC is for such an optimized system. This new reduced value can now be used for designing the electrothermal desorption part of ESA system to reduce the operating costs (Kaldate, 2005).

A scale-up model of the ESA system was developed by Kaldate (2005) by incorporating the experimental results obtained from this work. The decision variables were thickness of ACFC cloth, cartridge length, adsorption cycle time, desorption cycle time, cartridge aspect ratio, specific power requirement, maximum heating temperature, final oxygen concentration in vessel, and heating time during desorption. There were constraints on system parameters for the industrial application, such as diameter and length of the vessel. There are also constraints on other system parameters such as packing density, superficial gas velocity and system pressure drop (Kaldate, 2005). The objective function for optimization was energy per unit mass of the liquid recovered (e.g.
J/g). A summary of typical constraints and optimum values for a gas flow rate of 4,000 ft$^3$/min and MEK concentration of 525 ppmv is provided in Table 3-6.

Table 3-6. Constants for Decision Variables and Optimal Values for Air Stream Flow Rate of 4,000 ft$^3$/min and MEK Concentration of 525 ppmv (Kaldate, 2005)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Constraint</th>
<th>Optimal value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cloth thickness</td>
<td>0.005-0.1 cm</td>
<td>0.005</td>
</tr>
<tr>
<td>Cartridge length</td>
<td>1-400 cm</td>
<td>400.0</td>
</tr>
<tr>
<td>Adsorption cycle time</td>
<td>Desorption cycle time -240 min</td>
<td>106.7</td>
</tr>
<tr>
<td>Desorption cycle time</td>
<td>30-120 min</td>
<td>30.0</td>
</tr>
<tr>
<td>Cartridge aspect ratio</td>
<td>5-20</td>
<td>13.03</td>
</tr>
<tr>
<td>Maximum power</td>
<td>3-8 W/g ACFC</td>
<td>4.11</td>
</tr>
<tr>
<td>Maximum heating temperature</td>
<td>223-307 °C</td>
<td>279.6</td>
</tr>
<tr>
<td>Heating time</td>
<td>120-480 sec</td>
<td>244.5</td>
</tr>
<tr>
<td>Final oxygen concentration in the vessel</td>
<td>3-9%</td>
<td>4.87</td>
</tr>
</tbody>
</table>

A ranking analysis was done by Kaldate (2005) to compare the ESA technology with other competing technologies. In this analysis two other main competing technologies, granular activated carbon (GAC) adsorption and a thermal incinerator (TI) were considered along with optimal design of the ESA as presented in Table 3-6. Based on this analysis, TI has lower rank than adsorption technology due to use of large amounts of natural gas. GAC has lower capital costs ($245,900) and larger environmental impact (9,801 Pt) than for ESA ($280, 700 & 6,808 Pt).

The results and analysis provided in this section was limited to the single component adsorption. However, pilot-scale field study has demonstrated encouraging results for multi-component adsorption (Ramirez et al., 2005c & 2006).
3.1.1.3. Comparison of VaPRRS at the Bench-Scale and Pilot-Scale

In this section breakthrough curves (BTCs), throughput ratio (TPR), length of unused bed (LUB), and energy consumption are compared between the bench-scale VaPRRS and a pilot-scale VaPRRS (Ramirez et al., 2009). The TPR is defined as:

\[
TPR = \frac{t_s}{t_{s0}} \quad \text{Eq 3-1}
\]

TPR describes the steepness of the breakthrough curve. Higher TPR values indicate a steeper curve, where transient mass-transfer limitations become less important.

The LUB indicates the effective fraction of the adsorbent that is not utilized when the adsorption cycle is stopped at 5% breakthrough and is defined as:

\[
LUB = 1 - \frac{m_s}{m_{\text{sat}}} \quad \text{Eq 3-2}
\]

Each vessel of the pilot-scale system has an internal volume of 168 L and contains four annular cartridges of ACFC. Each cartridge contains 500 g of ACFC and was mounted in the vessel using stainless-steel fittings.

BTCs for both systems were obtained and compare values for TPR and LUB values (Figure 3-9). For the bench-scale system, BTCs were performed with gas flow rates ranging from 5 slpm to 140 slpm, corresponding to superficial gas velocities of 0.35 cm/sec and 9.7 cm/sec, respectively, and inlet MEK concentrations ranging from 100 ppmv to 10,000 ppmv. For the pilot-scale system, BTCs were performed with an air flow rate of 1.7 m$^3$/min (superficial gas velocity = 7.2 cm/sec) and inlet MEK vapor concentration ranging from 73 ppmv to 1,000 ppmv. Dimensionless BTCs from the bench-scale and pilot-scale systems were reproducible and follow the same trend with asymmetrical shape regardless of the tested inlet adsorbate concentration and volumetric air flow rate (Figure 3-9). For the bench-scale system, all BTCs start to rise in the range of $t/t_{s0}$ (actual duration of BTC test/duration of BTC at 50% breakthrough) from 0.75 to
0.9 with a steep slope, and they start to level off at $t/t_{50}$ of 1.4 and $C/C_0$ above 0.9. For the pilot-scale system, the behavior is similar with BTCs started to rise at $t/t_{50}$ of 0.65 with a steep slope that started to level off at $t/t_{50}$ of 1.2 and $C/C_0$ above 0.75 to 0.9.

Figure 3-9. Dimensionless Breakthrough Curves for the Bench-Scale and Pilot-Scale Systems

TPR and LUB values obtained from the BTC tests performed in the bench-scale and pilot-scale adsorber systems are provided in Figure 3-10. TPR values are 0.8±0.09 (mean ± standard deviation) and 0.7±0.05 for the bench-scale and pilot-scale systems, respectively. LUB average and standard deviation values are 0.2±0.11 and 0.3±0.07 for the bench-scale and pilot-scale systems, respectively. These values meet the minimum acceptable TPR value of 0.7 and a maximum acceptable LUB value of 0.3 as recommended by Sullivan (2001). The systematic difference between LUB and TPR (LUB=1-TPR) can be explained from the fact that the ratio of $m_{5\%}/m_{\text{sat}}$ is very close to the ratio of $t_{5\%}/t_{50\%}$, because breakthrough curve is almost symmetrical.
For the pilot-scale unit, the electrical energy consumed during each ACFC regeneration cycle was $1.7 \times 10^4$ kJ (19.4 kJ/g of ACFC) and $4.1 \times 10^4$ kJ (46.8 kJ/g of ACFC) for 170 ppmv and 940 ppmv of inlet MEK gas stream, respectively. The electrical energy per unit mass of recovered liquid MEK decreased from 25.9 kJ/g to 10.7 kJ/g as the MEK’s inlet concentration increased from 170 ppmv to 940 ppmv, respectively. Similarly, the electrical energy per unit mass of MEK adsorbed onto the ACFC cartridges decreased from 16.7 kJ/g to 7.2 kJ/g as the MEK concentration increased from 170 ppmv and 940 ppmv, respectively. The difference between the electrical energy per mass MEK recovered and the electrical energy per unit mass adsorbed for these two inlet concentrations ranges from 33% to 36%. The difference is caused by the liquid recovery efficiency (LRE) values < 100%. For the bench-scale system at 250 ppmv MEK inlet concentration the electrical energy consumption during each regeneration cycle of the ACFC was 0.73 kJ/g of ACFC, 4.57 kJ/g of liquid MEK recovered, and 4.15 kJ/g of MEK adsorbed. In contrast, the bench-scale system at 800 ppmv MEK inlet concentration the electrical energy consumption during each regeneration cycle of the ACFC was 0.72 kJ/g of ACFC, 4.84 kJ/g of liquid MEK recovered, and 4.39 kJ/g of MEK adsorbed (Figure 3-11).
The isosteric heat of adsorption describes the minimum energy required to desorb an adsorbate from the adsorbent. The isosteric heat of adsorption for MEK is 0.7 kJ/g (Ramirez et al., 2001). From the results in Figure 3-11, the total energy per unit mass of recovered condensate and the total energy per unit mass of MEK adsorbed are 15 and 10 times higher than the isosteric heat of adsorption for 940 ppmv of MEK, respectively. When the inlet concentration is lower (i.e., 170 ppmv) the difference is greater, which suggests that a significant quantity of the total energy applied to the system was used for heating other components inside the vessel such as fittings (Sullivan 2003).

3.1.1.4. Scale-Up of VaPRRS

Detailed descriptions of the scale-up of VaPRRS from bench-scale (100 slpm treated gas stream) to full-scale (57 actual m³/min) is out of scope of this research, however a summary of the calculation procedure to determine the mass of ACFC adsorbent, thickness of the cartridges, number of layers of cloth, and the resulting pressure drop, power (P), voltage (V), and current (I) requirements is provided here:
a) Mass of ACFC adsorbent:

The mass of adsorbent is estimated by:

\[ m_{ACFC} = \frac{\zeta m_s}{LUB q_{sat}} \]  

Eq 3-3

where \( m_s \) is described by:

\[ m_s = QC_{A, in} MW_{A} t_{ads} \]  

Eq 3-4

b) Thickness of cartridges and number of layers of cloth:

The outer radius of the cartridges is described by:

\[ r_o = \left( \frac{m_{ACFC}}{mn_{evlp} \left( -e \frac{1}{2} L \right) + r_i^2} \right)^{1/2} \]  

Eq 3-5

The thickness of the cartridge is then calculated by subtracting \( r_i \) from \( r_o \), the inner radius of the cartridge. The number of layers of cloth per cartridge is described by the thickness of cartridge divided by thickness of one layer of cloth:

\[ n_i = \frac{r_o - r_i}{t_{ACFC}} \]  

Eq 3-6

c) Pressure drop

Pressure drop is estimated from following equation:

\[ \Delta P = \frac{\mu_g}{\alpha} \frac{mQ_g}{2\pi nL} \ln \left( \frac{r_o}{r_i} \right) + \frac{\rho_g CmQ_g^2}{8\pi n^2 L^2} \left( \frac{1}{r_i} - \frac{1}{r_o} \right) \]  

Eq 3-7

d) Power, voltage, and current requirements

Total power (P) requirement is the power required per unit mass of cloth (\( \dot{P} \)) multiplied by the total mass of cloth:
Voltage (V) and current (I) requirements for each electrical circuit are described by:

\[ V = \left( \frac{P \cdot R}{n_e} \right)^{1/2} \]  
\[ I = \frac{P}{n_e V} \]

Where:

\[ R = \text{total electrical resistance of each circuit} = \frac{n_s R_c}{n_p} \]  
\[ R_c = \text{electrical resistance of each cartridge} = \rho_e \frac{L}{A_{\text{eff}}} \]  
\[ A_{\text{eff}} = \text{effective cross sectional area of each cartridge} = \frac{m_{\text{ACFC}}}{m \rho_f L} \]

3.1.2. ESA-SST

The steady-state tracking (SST) desorber was tested with three compounds: MEK, toluene and acetone. These organic vapors were selected based on their relevance to air quality; they have a wide range of boiling points 57°C to 111°C for relevant organic vapors, and their chemical structure existing as an aromatic or a ketone (Table 3-7).
Table 3-7. Selected Organic Compounds for SST Tests

<table>
<thead>
<tr>
<th>Organic compound</th>
<th>Chemical group</th>
<th>Chemical structure</th>
<th>Boiling point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetone</td>
<td>Ketone</td>
<td><img src="image" alt="Acetone Structure" /></td>
<td>56.5</td>
</tr>
<tr>
<td>Methyl ethyl ketone</td>
<td>Ketone</td>
<td><img src="image" alt="Methyl Ethyl Ketone Structure" /></td>
<td>80</td>
</tr>
<tr>
<td>Toluene</td>
<td>Aromatic</td>
<td><img src="image" alt="Toluene Structure" /></td>
<td>111</td>
</tr>
</tbody>
</table>

SST tests were performed at low concentration (500 ppmv) which is appropriate for treatment with biofilters, and high concentration (5,000 ppmv) which is appropriate for treatment with thermal oxidizers. In order to demonstrate the performance of an SST system at the conditions where set-point and flow rate might need to change with time, dynamic-tracking desorption was also tested with carefully controlled yet variable vapor concentrations ranging between 250 ppmv and 5,000 ppmv, while also allowing the flow rate of the carrier gas to change by 100%. Finally the SST system was tested for cyclic operation which is applicable for continuous operation.

3.1.2.1. Low Concentration Tests

In this section the results for SST desorption at 500 ppmv MEK outlet concentration for the three mentioned organic compounds are presented. For each test a group of four graphs describe: 1) set-point and measured outlet concentrations, 2) average temperatures of the cartridges and vessel wall, 3) extent of measured regeneration and extent of regeneration if there was equilibrium between vapor phase and adsorbed phase, and 4) power and total energy consumed for a regeneration cycle. The first graph demonstrates the performance of the PID controller to control the organic vapor’s outlet concentration during regeneration tests based on the defined PID set-point. The second graph shows the
thermal history of the cartridge and vessel wall. It is important to measure the cartridge temperature to assure that damage does not occur to the adsorbent. The third plot is important because it describes the extent of regeneration that is limited by the thermal decomposition of the adsorbent in air. The fourth plot is important because it describes how power applied to the cartridges increases with decreasing loading of the adsorbate in the ACFC and is also important in designing an appropriate electrical circuit to regenerate the adsorbent. For example, total energy consumption is an important factor when considering operating costs.

The measured MEK concentration at the outlet of the vessel, the corresponding set-point concentration of 500 ppmv, the temperatures of the cartridges and vessel, $\eta_{\text{reg}}$ and $\eta_{\text{reg,eq}}$, and $\dot{Q}_{e,m}$ and $\dot{Q}_{e,c}$ during SST desorption tests are described in Figure 3-12A through Figure 3-12D, respectively. The measured MEK outlet concentration was 496±3 ppmv. The AAE between the set-point and the measured MEK concentration was 0.94%. Temperature of the adsorbent increased from 25°C to 100°C because of the additional energy applied to the cartridges to maintain the constant outlet MEK concentration despite the reduction in the amount of adsorbed MEK as time lapsed during the test. The AAE of 20% between $\eta_{\text{reg}}$ and $\eta_{\text{reg,eq}}$ is most likely due to the assumption of equilibrium between vapor-phase and adsorbed phase, possible heterogeneity within the adsorbent, error in the temperature measurement, and use of the exponential sensitivity of the DR equation to temperature when describing $\eta_{\text{reg,eq}}$ (Figure 3-12C). Assuming equilibrium conditions should be reasonable due to the ACFC’s small fiber diameter of 12.3±1 μm (Lo, 2002). However, adsorbate loading and temperature may not be uniformly distributed in the cartridges. Also, the DR equation has an AAE ≤ 9.2% when comparing measured and modeled equilibrium adsorption capacities for the ACFC-MEK system between 20°C and 175°C (Ramirez, 2004). The average $\dot{Q}_{e,m}$ value was 15.5 W resulting in an energy per unit mass of desorbed MEK of 28.6 kJ/g. Energy consumption is an important part of operating cost. It increases with gas flow rate and extent of regeneration. Decreasing the extent of regeneration will lower the energy consumption; however it will increase the amount of required ACFC. Optimization needs to be
performed in order to minimize the overall system cost while maximizing the performance of the system.

SST tests at an outlet set-point concentration of 500 ppmv were also performed with acetone and toluene and are shown in Figure 3-13 and Figure 3-14, respectively. A summary of results for the three organic compounds is provided in Table 3-8. The AAE between the set-point and the measured organic vapor concentrations were < 1.1%. Energy per unit mass of desorbed organic vapor when 80% of the adsorbate was removed from the ACFC (to compare similar conditions for the tests) was highest for toluene (35.3 kJ/g) and lowest for acetone (14.7 kJ/g). That is because acetone has the lowest boiling point resulting in desorption of acetone at lower temperatures. Consequently energy consumed to heat the cloth, air stream, tubes, and plugs is lower for acetone.
A- The vessel’s outlet vapor concentration with a set-point of 500 ppmv

B- Temperature of the ACFC and the vessel wall

C-Extent of regeneration of the ACFC

D-Power and cumulative energy deposited to the ACFC

Figure 3-12. Steady-State Desorption Test Results to Achieve a MEK Concentration of 500 ppmv in 20 slpm Air
A- The vessel’s outlet vapor concentration with a set-point of 500 ppmv

B- Temperature of the ACFC and the vessel wall

C- Extent of regeneration of the ACFC

D- Power and cumulative energy deposited to the ACFC

Figure 3-13. Steady-State Desorption Test Results to Achieve an Acetone Concentration of 500 ppmv in 20 slpm Air
A- The vessel’s outlet vapor concentration with a set-point of 500 ppmv

B- Temperature of the ACFC and the vessel wall

C- Extent of regeneration of the ACFC

D- Power and cumulative energy deposited to the ACFC

Figure 3-14. Steady-State Desorption Test Results to Achieve a Toluene Concentration of 500 ppmv in 20 slpm Air
### Table 3.8. SST Experimental Test Results at 500 ppmv for Three Organic Compounds

<table>
<thead>
<tr>
<th>Adsorbate</th>
<th>Average Concentration (ppmv)</th>
<th>Standard Deviation (ppmv)</th>
<th>AAE (%)</th>
<th>Cartridge temperature at 80% desorption</th>
<th>Average Energy per unit mass of adsorbate desorbed at 80% desorption (kJ/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MEK</td>
<td>496</td>
<td>3</td>
<td>0.94</td>
<td>102</td>
<td>28.6</td>
</tr>
<tr>
<td>Acetone</td>
<td>494</td>
<td>6</td>
<td>1.1</td>
<td>55</td>
<td>14.7</td>
</tr>
<tr>
<td>Toluene</td>
<td>498</td>
<td>1</td>
<td>0.37</td>
<td>111</td>
<td>35.3</td>
</tr>
</tbody>
</table>

#### 3.1.2.2. High Concentration Tests

Desorption of MEK at a constant set-point of 5,000 ppmv resulted in a measured MEK outlet concentration of 4,962±32 ppmv and an AAE of 0.8% between these two parameters (Figure 3-15). Maximum temperature of the adsorbent was 152°C, which is 52°C more than the test at 500 ppmv MEK because more power was required to achieve a faster rate of desorption to obtain the higher set-point concentration. The average $\dot{Q}_{e,m}$ value was 25.8 W resulting in an energy per unit mass value of desorbed MEK of 9.9 kJ/g. Although more power is required at a higher outlet concentration, the duration of the desorption cycle is less, and the electrical energy is 65% less than for the 500 ppmv case. Discussion about the distribution of energy during each desorption cycle is described later.

For safety considerations, an alarm was set in the control system for the gas temperature to remain below a specified value to keep the gas stream’s organic vapor concentration below its lower flammable limit (LFL). It’s important to keep the concentration of flammable vapors below their LFL value if the regeneration cycle occurs with sufficient oxygen to sustain a flame. The LFL value for MEK concentration in air is calculated by:

$$LFL_T = LFL_{25^\circ C} \left[1 - \frac{0.75 (T - 25)}{\Delta H_C}\right]$$

Eq 3-14

where $T$ is the temperature of the air (°C), $\Delta H_C$ is the net heat of combustion (kcal/mol),
and the subscripts define the temperature for the LFL of MEK vapor in air. The maximum temperature during all of the desorption tests was 156°C. The LFL at this temperature is 14,773 ppmv, which is 200% higher than the maximum MEK set-point concentration of 5,000 ppmv. It should be noted that MEK concentration is higher within the ACFC’s pores than the bulk gas, but the maximum temperature experienced by the adsorbent was less than the auto-ignition temperature of 514°C for the bulk MEK concentration in air, and no fires were observed during the regeneration tests.

SST tests at 5,000 ppmv were also performed with acetone and toluene and are shown in Figure 3-16 and Figure 3-17. A summary of results for the three organic compounds is provided in Table 3-9. The AAE between the set-point and the measured organic vapor concentration was < 1.9% for all three tests. Energy per unit mass of desorbed organic vapor when 80% of the adsorbate was removed from the ACFC (to compare similar conditions for the tests) was highest for acetone (14.6 kJ/g) and lowest for MEK (9.9 kJ/g). As previously reported, acetone has the lowest boiling point, but since its adsorption capacity on ACFC is low compared to toluene and MEK, the consumed energy per unit mass of desorbed acetone is high compared to two toluene and MEK.
A- The vessel’s outlet vapor concentration with a set-point of 500 ppmv

B- Temperature of the ACFC and the vessel wall

C- Extent of regeneration of the ACFC

D- Power and cumulative energy deposited to the ACFC

Figure 3-15. Steady-State Tracking Desorption Test Results to Achieve an MEK Outlet Concentration of 5,000 ppmv at 10 slpm in Air
A- The vessel’s outlet vapor concentration with a set-point of 500 ppmv

B- Temperature of the ACFC and the vessel wall

C- Extent of regeneration of the ACFC

D- Power and cumulative energy deposited to the ACFC

Figure 3-16. Steady-State Desorption Test Results to Achieve an Acetone Concentration of 5,000 ppmv in 10 slpm Air
A- The vessel’s outlet vapor concentration with a set-point of 500 ppmv

B- Temperature of the ACFC and the vessel wall

C- Extent of regeneration of the ACFC

D- Power and cumulative energy deposited to the ACFC

Figure 3-17. Steady-State Desorption Test Results to Achieve a Toluene Concentration of 5,000 ppmv in 10 slpm Air
Table 3-9. SST Experimental Test Results at 5,000 ppmv for three Organic Compounds

<table>
<thead>
<tr>
<th>Adsorbate</th>
<th>Average Concentration (ppmv)</th>
<th>Standard Deviation (ppmv)</th>
<th>AAE (%)</th>
<th>Cartridge temperature at 80% desorption</th>
<th>Average Energy per unit mass of adsorbate desorbed at 80% desorption (kJ/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MEK</td>
<td>4,962</td>
<td>32</td>
<td>0.8</td>
<td>117</td>
<td>9.9</td>
</tr>
<tr>
<td>Acetone</td>
<td>4,908</td>
<td>81</td>
<td>1.9</td>
<td>106</td>
<td>14.6</td>
</tr>
<tr>
<td>Toluene</td>
<td>4,954</td>
<td>26</td>
<td>0.96</td>
<td>154</td>
<td>12.2</td>
</tr>
</tbody>
</table>

3.1.2.3. Dynamic Tests

Results from the dynamic SST outlet concentration tests at two air flow rates demonstrate that the system is very responsive at controlling the concentration of MEK based on the set-points with an AAE between the measured and set-point concentrations of 2.8% (Figure 3-18A). The sharp spikes in the middle of the plots in Figure 3-18 are due to the specified air flow rate increasing by 100% and the change in the dilution ratio for the PID. However, the controller quickly responded to return the outlet MEK concentration to its set-point value. The temperature of the cartridges ranged between 25°C and 112°C as \( \dot{Q}_{e,m} \) increased or decreased between 1.0 W and 84 W. The average \( \dot{Q}_{e,m} \) was 22 W resulting in an energy per unit mass of desorbed MEK of 9.2 kJ/g.
Figure 3-18. Dynamic Tracking Desorption Test Results to Achieve MEK Outlet Concentrations Between 500 ppmv and 5,000 ppmv at 10 slpm and 20 slpm in Air
3.1.2.4. Cyclic Tests

Cyclic adsorption/desorption test was performed with adsorption of MEK vapor at 500 ppmv in 100 slpm air and then desorption at 5,500 ppmv and 10 slpm air as it is shown in Figure 3-19. The temperature of the cartridges ranged between 25°C and 160°C as $\dot{Q}_{e,m}$ increased or decreased between 13.5 W and 60 W. Average extent of desorption was 90%. These tests demonstrate that the bench-scale system can continuously treat an air stream containing MEK while operating repetitively and consistently without operator intervention.
A- The vessel’s outlet vapor concentration with a set-point of 500 ppmv

B- Temperature of the ACFC and the vessel wall

C- Extent of regeneration of the ACFC

D- Power and cumulative energy per cycle deposited to the ACFC

Figure 3-19. Cyclic Steady-State Desorption Test Results to Achieve a MEK Concentration of 5,500 ppmv in 10 slpm Air from MEK Concentration of 500 in 100 slpm Air
These results demonstrate that SST desorption can be used to regenerate ACFC at much lower gas flow rate than during the adsorption cycle with a carefully controlled vapor concentration that can be efficiently treated by an oxidizer at thousands of ppmv or a biofilter at hundreds of ppmv. Successfully tested concentration ratios (adsorption concentration/desorption concentration) ranged from 0.1 to 1. Such capabilities are very important because many of the sources of HAPs/VOCs (e.g., coating operations) have highly variable vapor concentrations (+110%) at very high gas flow rates (~300 m³/min). SST desorption readily stabilizes the vapor concentration (+1%) and independent control of gas flow rate and regeneration power provides robust control of low-flow-rate effluent gas streams. SST can reduce the gas flow rate to <10% of the original gas flow rate before further treatment by an oxidizer or biofilter.

3.1.2.5. Concomitant Adsorption and Desorption in Dry and Humid Air Streams

Conditions that existed for the CAD tests while treating a dry air stream (ESA₁), and a humid air stream (ESA₂) are described in Table 3-10. These conditions were defined to provide variable inlet organic vapor concentrations (i.e., MEK), a constant outlet organic vapor concentration, and to test the impact of high humidity (multi-component vapor as the inlet gas stream) to test the ability of ESA to provide a constant outlet organic vapor concentration. The results are provided in Figure 3-20 and Figure 3-21.

The resulting inlet, outlet, and the set-point organic vapor concentrations are provided in Figure 3-20 (A) for the dry inlet gas stream and the same parameters plus the inlet RH values are provided in Figure 3-21 (A) for the humid inlet gas stream. Corresponding AAE values between the measured outlet organic vapor concentrations and the set-point organic vapor concentrations were very encouraging at 0.4% (ESA₁), and 0.3% (ESA₂). The ability for the ESA-CAD system to readily control the outlet MEK concentration is reflected by the small AAE values for dry and humid inlet gas streams.

The temperature profiles for the ACFC and the vessel’s wall for both systems are described in Figure 3-20 (B) and Figure 3-21 (B). The fluctuation in the ACFC’s temperature reflects the application of power to the ACFC. The cartridge temperature quickly reached a steady-state value between 48°C and 55°C. These values are much
lower than demonstrated for the SST desorption tests where the temperature continued to increase to 150°C by the end of the regeneration tests (Emamipour et al., 2007; Hashisho et al., 2007). The differences in temperature trends is due to the replenishment of organic vapor to the ACFC by the inlet gas stream for the CAD tests that did not occur for the SST tests. The temperature of ACFC needed to be increased during the SST test because the reservoir of adsorbed MEK was depleting with time, unlike the condition for the CAD tests where the loading of MEK onto the adsorbent varied periodically.

Table 3-10. Summary of CAD Operating Parameters for ESA

<table>
<thead>
<tr>
<th>Parameter</th>
<th>ESA₁</th>
<th>ESA₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet concentrations (ppmv)</td>
<td>1-500</td>
<td>1-530</td>
</tr>
<tr>
<td>Average inlet concentration (ppmv)</td>
<td>250</td>
<td>265</td>
</tr>
<tr>
<td>Air flow rate (slpm)</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>Inlet RH (%)</td>
<td>&lt; 2</td>
<td>85</td>
</tr>
<tr>
<td>Outlet set-point concentration (ppmv)</td>
<td>250</td>
<td>250</td>
</tr>
<tr>
<td>Average outlet concentration (ppmv)</td>
<td>250.0</td>
<td>250.1</td>
</tr>
<tr>
<td>AAE (%)</td>
<td>0.4</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Adsorption of water vapor on ACFC depends on \( T_c, C_{\text{water}}/C_{\text{water}}^* \) (= RH (%)/100), and \( C_{\text{MEK}}/C_{\text{water}} \).

Where:

\( T_c = \) temperature of cartridge = 49°C

\( C_{\text{water}} = \) concentration of water vapor = 1.09 (mol/m³)
Figure 3-20. CAD Test Results to Achieve MEK Outlet Concentration of 250 ppmv at 20 slpm in Dry Air
A- The vessel’s inlet and outlet organic vapor concentrations and the inlet gas stream’s RH with a set-point of 250 ppmv for the outlet organic vapor concentration

B- Temperature of the ACFC and the vessel wall

C- Mass balance of organic vapor

D- Power and cumulative energy per cycle deposited to the ACFC

Figure 3-21. CAD Test Results to Achieve MEK Outlet Concentration of 250 ppmv at 20 slpm in Humid Air
$C_{\text{water}}^*$ = saturation concentration of water vapor in air = 4.36 (mol/m$^3$)

$C_{\text{MEK}}$ = concentration of MEK vapor = 0.018 (mol/m$^3$)

$C_{\text{water}}/C_{\text{water}}^*$ of the inlet gas stream for the ESA$_2$ test was 0.85 (RH = 85%); however as the air stream approaches the heated ACFC cartridge, the air’s dry-bulb temperature increases at a constant dew-point temperature, and the local value of $C_{\text{water}}/C_{\text{water}}^*$ is lowered due to the increase in $C_{\text{water}}^*$ with increasing dry-bulb temperature. Assuming the air stream has the same temperature as the ACFC cartridge when it passes between the fibers of the ACFC cartridge (49°C) results in $C_{\text{water}}/C_{\text{water}}^*$ = 0.25 (RH = 25%) for the gas stream.

The adsorption isotherm of water vapor on ACFC is Type V. This isotherm type is characterized by low adsorption capacity at low RH values (< 40% RH) followed by a sharp increase and then a plateau with little further increase in adsorption capacity with increasing RH values (Figure 3-22). In contrast, MEK adsorption on ACFC exhibits a Type I isotherm. As the relative pressure of the organic vapor initially increases, there is a rapid increase in adsorption capacity until the adsorption capacity levels off asymptotically and approaches the micropore volume of the ACFC. Hence, a mild increase in temperature (20°C - 30°C) has a larger effect on reducing the adsorption capacity of water vapor (Type V isotherm) then for organic vapor (Type I isotherm).

At 25°C, the equilibrium adsorption capacity of water vapor on ACFC-20 is < 0.01 g H$_2$O/g of ACFC at RH = 25% (Cal et al., 1997; Sullivan et al., 2007). At 49°C, the adsorption capacity is expected to be even lower. Although adsorption competition between water vapor and MEK is a function of MEK’s and water vapors' relative pressures, competitive adsorption by water vapor on ACFC at these conditions is expected to be insignificant. Hence, at the heated cartridge temperature, the water vapor is not adsorbed but penetrates through the adsorbent.
Figure 3-22. Adsorption Isotherms for MEK and H₂O at 25°C and 50°C on ACFC-20. Solid lines are obtained using Dubinin–Radushkevich equation and data from (Ramirez et al., 2004). Symbols describe MEK data (Ramirez et al., 2004) and Water data (Sullivan et al., 2007).

The mass of MEK adsorbed to the ACFC was determined with a mass balance by taking the difference between the MEK entering and exiting the vessel as described in Figure 3-20 (C) and Figure 3-21 (C). The cumulative mass of MEK entering the vessel increased stepwise reflecting the variation in the inlet concentration between the specified low and high inlet MEK concentrations. The cumulative mass of MEK emitted from the vessel increased linearly with time since the total gas flow rate and the outlet MEK concentration were constant. The amount of MEK adsorbed to the ACFC varied within a narrow limit (within 5% for ESA₁), and (within 3% for ESA₂) as demonstrated in Figure 3-20 (C) and Figure 3-21 (C). The amount of MEK adsorbed is important for sustainable operation of the CAD system since having an excessive amount of adsorbed MEK will diminish the adsorption capacity of the ACFC and result in an outlet concentration that is higher than the desired set-point concentration. However, having insufficient adsorbed MEK will require higher power application and energy consumption to desorb the MEK to sustain the vessel’s desired outlet set-point concentration. If all of the MEK is desorbed, then the system will not provide the desired target outlet concentration for
stable operation of the secondary device (e.g., downstream biofilter). Hence, the design of a CAD system needs to take into consideration the strength of the emission source, and the concentration of organic vapor needed for the optimum operation of the secondary device (e.g., biofilter).

The power and cumulative energy deposited to the ACFC during the CAD tests are described in Figure 3-20 (D) and Figure 3-21 (D). Initially, the power deposited to the ACFC cartridges quickly increased since the cartridges need to be heated above ambient conditions to desorb MEK and match the set-point MEK concentration for the outlet gas stream. The power then quickly reached a steady-state level with an average value of 14.5 W (ESA₁), and 14.2 W (ESA₂) which corresponds to 55 kJ/g (ESA₁), and 53 kJ/g (ESA₂) of MEK desorbed. The cumulative energy during the CAD tests increased linearly with time since power deposition didn’t depend more on the set-point of the organic vapor’s outlet concentration than on the fluctuating in inlet concentration for the conditions tested here. The amount of energy deposited to the ACFC per unit mass of MEK desorbed during CAD operation is larger than the corresponding values during SST tests (9-29 kJ/g) for the conditions reported here. This observation is due to the systems’ operating conditions, with the SST system typically experiencing lower carrier gas flow rates and higher adsorbate concentrations than for the corresponding CAD system. The power consumption for the ESA₁ (dry) and ESA₂ (humid) were comparable since a negligible amount of water vapor adsorbed onto the ACFC. While power consumption was higher for CAD operation when compared to SST operation of the ESA systems, CAD systems can operate continuously with a single vessel, while a SST system needs at least two vessels for continuous dampening of concentration fluctuations. Since desorption occurs after adsorption with SST systems, the gas flow rate during desorption can be smaller than the gas flow rate during adsorption and results in a smaller secondary control device (e.g., volume of biofilter). However, during CAD operation of the ESA system there is concomitant adsorption and desorption at a constant gas flow rate. Such constant flow rate is expected to result in a larger downstream biofilter when compared to a SST system. However, both devices are expected to allow for more effective operation of a biofilter to dispose of organic vapors in gas streams.
This work does not include performance analysis of an integrated CAD-biofilter, but describes the ability to readily stabilize the concentration of an organic vapor in a gas stream that has a highly unstable organic vapor concentration. The resulting gas stream can then be more readily treated by a secondary control device such as a biofilter. Future work needs to provide an economic analysis of implementing CAD and a performance analysis of the biofilter with and without using CAD and SST systems.

### 3.1.2.6. Energy Distribution

The distributions of deposited energy once 80% of the MEK was desorbed from the ACFC were determined with the equations described in Table 3-11 and is shown in Figure 3-23. Descriptions of the parameters used in the equations are provided in Table 3-12. Note that, the vessel’s wall is heated by the air stream and radiation from the cartridges and is cooled down from the other side by the ambient air. However, the control volume for the energy balance is taken around the cartridges, therefore, only heat exchange between the vessel’s wall and the cartridges must be included in the energy balance.

**Table 3-11. Equation Used for Calculation of Energy Distribution**

<table>
<thead>
<tr>
<th>Energy term</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air-sensible heat</td>
<td>$Q_{reg} P^o M_{Air} \frac{T}{R T^o} c_{p,air} dT$</td>
</tr>
<tr>
<td>Convection</td>
<td>$h_c A_c (T - T_w)$</td>
</tr>
<tr>
<td>Radiation</td>
<td>$\frac{\sigma (T^4 - T_w^4)}{\varepsilon_w A_c + \frac{1}{A_c F_{c-w}} + \frac{\varepsilon_w}{\varepsilon_w A_w}}$</td>
</tr>
<tr>
<td>Fittings-sensible heat</td>
<td>$m_{fitings} c_{p,fitings} \frac{dT}{dt}$</td>
</tr>
<tr>
<td>Liquid adsorbate-(sensible heat + heat of desorption)</td>
<td>$m_{MEK} c_{p,MEK} \frac{dT}{dt} + \Delta H_{ads} m_{MEK}$</td>
</tr>
<tr>
<td>ACFC-sensible heat</td>
<td>$m_{ACFC} c_{p,ACFC} \frac{dT}{dt}$</td>
</tr>
</tbody>
</table>
Table 3-12. Parameters Used for the ESA-SST System’s Energy Balance

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m_{ACFC} )</td>
<td>73.53</td>
<td>G</td>
</tr>
<tr>
<td>( c_{p,ACFC} )^{a}</td>
<td>0.971^{(III)}</td>
<td>J g(^{-1}) K(^{-1})</td>
</tr>
<tr>
<td>( m_{MEK} )</td>
<td>f(t)</td>
<td>G</td>
</tr>
<tr>
<td>( c_{p,MEK} )</td>
<td>2.19^{(I)}</td>
<td>J g(^{-1}) K(^{-1})</td>
</tr>
<tr>
<td>( m_{fittings} )</td>
<td>366</td>
<td>G</td>
</tr>
<tr>
<td>( c_{p,fittings} )</td>
<td>0.47^{(III)}</td>
<td>J g(^{-1}) K(^{-1})</td>
</tr>
<tr>
<td>( T )</td>
<td>f(t)^{b}</td>
<td>K</td>
</tr>
<tr>
<td>( M_{air} )</td>
<td>28.97</td>
<td>g-mol(^{-1})</td>
</tr>
<tr>
<td>( T_{in} )</td>
<td>25</td>
<td>K</td>
</tr>
<tr>
<td>( c_{p,air} )</td>
<td>f(T)</td>
<td>J g(^{-1}) K(^{-1})</td>
</tr>
<tr>
<td>( h_{e} )</td>
<td>f(T)^{I}</td>
<td>W m(^{-2}) K(^{-1})</td>
</tr>
<tr>
<td>( A_{e} )</td>
<td>0.039</td>
<td>m(^{2})</td>
</tr>
<tr>
<td>( T_{w} )</td>
<td>f(t)</td>
<td>K</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>5.667x10(^{-8})</td>
<td>W m(^{-2}) K(^{-4})</td>
</tr>
<tr>
<td>( \varepsilon_{ACFC} )</td>
<td>0.9^{(I)}</td>
<td>-</td>
</tr>
<tr>
<td>( \varepsilon_{w} )</td>
<td>0.09^{(II)}</td>
<td>-</td>
</tr>
<tr>
<td>( F_{c-w} )</td>
<td>0.922</td>
<td>-</td>
</tr>
<tr>
<td>( A_{w} )</td>
<td>0.0982</td>
<td>m(^{2})</td>
</tr>
<tr>
<td>( \Delta H_{ads} )</td>
<td>700^{(IV)}</td>
<td>J g(^{-1})</td>
</tr>
<tr>
<td>( \dot{m}_{MEK} )</td>
<td>f(t)</td>
<td>g s(^{-1})</td>
</tr>
</tbody>
</table>

\(^{a}\) Same as graphite; \(^{b}\) Varies with time

\(^{I}\)Sullivan (2004); \(^{II}\)Holman (1981); \(^{III}\)Millas (1999); \(^{IV}\)Ramirez (2005)
Sensible heat for the gas is the largest energy term (49% to 76%), as it increased with decreasing temperature and decreasing MEK outlet concentration, but increased with increasing duration of the desorption cycle. Convection energy was the distant second largest term (10% to 18%), as it increased with increasing temperature and increasing MEK concentration, but decreased with increasing duration of the desorption cycle.

Total deposited energy for the SST desorption at 5,000 ppmv is lower than 500 ppmv because of shorter desorption time and lower gas flow rate. Majority of energy is consumed to heat up the gas stream to about temperature of cloth at the outer surface of cartridges. Part of this energy can be recovered by using a heat exchanger between inlet and outlet gas stream in order to improve the thermal efficiency of the ESA-SST. This will also lower the temperature of outlet gas stream to be appropriate for destruction in biofilter.

![Energy Distribution for Steady State and Dynamic Tracking Desorption Tests](image)

A- Steady state tracking desorption with a set-point of 500 ppmv  
B- Steady state tracking desorption with a set-point of 5,000 ppmv  
C- Dynamic tracking desorption with set-points from 500 ppmv to 5,000 ppmv

Figure 3-23. Energy Distribution for Steady State and Dynamic Tracking Desorption Tests
3.2. Simulation Results and Comparison to Experimental Results

CFD simulations were developed and implemented to provide results that will hopefully allow for the use of more simplified 1-D modeling compared to much more complex 3-D modeling. Velocity profiles of the gas stream through the adsorbent and vessel were developed using 3-D simulations. Results from those simulations can then be used to evaluate the uniformity of these velocity profiles and if uniform velocity profiles can then be used to describe heat and mass transfer using 1-D models.

3.2.1. Computational Fluid Dynamics

3.2.1.1. Fluid Flow (Cylindrical Cartridge System)

Dependence of measured ΔP values on total gas flow rate between 10 alpm and 160 alpm through each of the four cartridges of ACFC are described in Figure 3-24. ΔP values for all four cartridges are not exactly the same because of differences in the mass of each cartridge and experimental error. The AAE between the measured and fitted ΔP values is 5%. The values of $\alpha = 1.70 \times 10^{-11} \text{ m}^2$ and $C = 1.76 \times 10^6 \text{ m}^{-1}$ were then determined by fitting Eq 2-8 to the ΔP data as shown in Figure 3-24. The regression coefficient ($R^2$) is 0.98. These values are the only fitted values in these simulations.

![Figure 3-24. Measured Pressure Drop (ΔP) of Four Individual ACFC Cartridges and Resulting Regression Line as a Function of Gas Flow Rate](image-url)
The computational mesh generated for the CFD simulation to model the ΔP and gas velocity patterns are provided in Figure 3-25. There isn’t significant gas flow through the bottom and top of the cartridges because those areas are blocked by their plugs and inlet tubes. Brackets (i.e., hose clamps) are considered to cause minimal disturbances to the gas flow. As such the brackets were not included in the simulation, which also simplified the computational mesh. The fitted values for $\alpha$ and C were then used in the CFD simulation to describe ΔP and gas velocity values as the air stream entered the vessel, passed from the inside to the outside of each cartridge for one pair of cartridges, passed through the interior of the vessel, then from the outside to the inside of each cartridge for a second pair of cartridges, and finally exited the vessel. It should be noted that values for $\alpha$ and C were obtained by fitting the Eq 2-8 to the pressure drop data of individual cartridges while simulation was performed for entire vessel containing four cartridges.

Figure 3-25. 3-D Geometry of the Adsorption Vessel (A) and Computational Mesh for the Cartridges

Comparison of ΔP values from the CFD simulations and measurements for the entire vessel, including the cartridges, is provided in Figure 3-26. The AAE values between simulated and measured ΔP values are < 1%. Note that values of $\alpha$ and C were obtained
from pressure drop data for an individual cartridge, while simulations were performed for the entire vessel containing four cartridges. The first pair of cartridges provided parallel gas flow through them and then a second pair of cartridges provided parallel gas flow to them, with gas flow occurring in series between the two pairs of cartridges.

Figure 3-26. Pressure Drop Data ($\Delta P$) from Physical Experiments and Simulations for the Entire Adsorption Vessel and the Four Cartridges (1 cm H$_2$O equals 98.06 Pa)

Contours of simulated $\Delta P$ values for a typical total gas flow rate of 50 slpm (superficial gas velocity of 1.46 m/s at the inlet tube of the vessel) indicate that $\Delta P$ caused by the cartridges is $> 99\%$ of the total $\Delta P$ across the vessel, which is 486.5 Pa (Figure 3-27A). The remaining $\Delta P$ is caused by the flow of gas through the vessel’s interior. The $\Delta P$ contours provided in Figure 3-27A are also described in Figure 3-27B; however, they are presented in a horizontal plane at the middle height of the cartridges and with greater resolution. The $\Delta P$ contours are uniform in the vertical and tangential directions of the cartridges, with uniformly increasing $\Delta P$ in the radial direction of gas flow within the cartridges.
The uniformity of $\Delta P$ values across the cartridges results in uniform gas velocity contours across the cartridges as described in the horizontal planes across the vessel and cartridges (Figure 3-28A). The dark blue sections at the top and bottom of the cartridges indicate that flow across those parts of the cartridges is very small, which is caused by the impervious brackets that mount the ACFC cartridges within the vessel. The same velocity magnitude contours described in Figure 3-28A are also described in Figure 3-28B; however, the results are presented in a horizontal plane at the middle height of the cartridges and with greater resolution. As with the $\Delta P$ contours, the velocity contours are uniform in the vertical and tangential directions of the cartridges. However, the radial velocity across the first set of cartridges decreases by 39% as the gas passes through the cartridges and it increases by the same amount as the gas passes through the second set of cartridges. Such velocity gradient is caused by the change in cross-sectional area of the annular cartridges as the gas flows through them.
The uniformity in velocity magnitudes is even more apparent when plotting gas velocity at the middle radius of the cartridges as a function of cartridge length and angle (Figure 3-29A). Gas velocity increases rapidly with respect to the cartridge’s length to its maximum value over the first 10% of the cartridge’s length, remains constant for the next 80% of the cartridge’s length, and then rapidly decreases to zero for the remaining 10% of the cartridge’s length. As previously mentioned, the reduction in the velocity’s magnitude at each end of the cartridge is caused by the impervious mounting brackets used to mount the cartridges in the vessel. The velocity profile within the first set of two cartridges is almost identical to the velocity profile within the second set of two cartridges. The only difference is that the radial gas velocity within the first set of cartridges is in the opposite direction (i.e., flowing from the inside to the outside of the cartridges and experiencing an increase in cross-sectional area) as the radial gas velocity within the second set of cartridges (i.e., flowing from the outside to the inside of the cartridges and experiencing a decrease in cross-sectional area) (Figure 3-29B).
3.2.1.2. Fluid Flow (Pleated Filter)

Another possible configuration of the ACFC is a pleated filter. Figure 3-30 shows the cross section of the filter from top view. The dimensions for the filter to treat a 200 ft³/min gas stream are 43 cm x 30 cm x 30 cm (17 in x 12 in x 12 in), with the 43 cm x 30 cm face exposed to the air stream. Overall thickness of the cloth material is 0.64 cm (0.25 in).
Contours of pressure and streamlines are demonstrated in Figure 3-31 and Figure 3-32, respectively. Similar to the cartridge configuration, it can be seen that the uniformity of $\Delta P$ values across the ACFC cloth results in uniform gas velocity contours across the ACFC cloth. $\Delta P$ caused by the ACFC cloth (740 Pa) is more than 99% of the total pressure drop across the entire assembly.

These results indicate that uniform velocity profiles exist for cylindrical and pleated filters at ambient temperature and pressure, superficial gas velocity in the pleated filter of 0.15 m/s, and superficial gas velocity in a cylindrical filter of 0.032 m/sec. However, results were not obtained to indicate when the velocity profiles become non-uniform for these two sets of conditions.
Figure 3-31. Contours of Pressure in the Pleated ACFC Assembly

Figure 3-32. Contours of Streamlines in the Pleated ACFC Assembly
3.2.1.3. *Fluid flow and heat transfer*

The computational mesh generated for the simulation of fluid flow and heat transfer is provided Figure 3-33.

![Computational Mesh for Simulation of Heat Transfer and Fluid Flow](image)

Figure 3-33. Computational Mesh for Simulation of Heat Transfer and Fluid Flow

Experimental and modeled temperature of cartridges at four locations (T1: 1.5 cm, T2: 5.75 cm, T3: 14.25 cm, and T4: 18.5 cm from bottom of cartridges) as a function of time for electrothermal heating with a nitrogen flow rate of 1 slpm and heating with hot air at 41.1 slpm and maximum inlet temperature of 260°C are provided in Figure 3-34 and Figure 3-35, respectively. Top and bottom of cartridges are colder than center because there is heat transfer to the tubes and plugs. Heating occurs much more rapidly with electrothermal heating with the experimental temperature of the cartridges achieving their maximum value of 200°C within 60 sec for electrothermal heating in contrast to 700 sec for hot air heating.

Distributions of the sum of the thermal energy terms at the end of the heating cycles are provided in Figure 3-36. Only 13% of consumed energy is being used for heating of
cartridges in hot air heating compare to 78% in electrothermal heating. More energy is transferred to the vessel wall by convection for hot air heating compared to electrothermal heating (20.2% vs. 3.7%, respectively) because the gas flow rate is higher for hot air heating compared to electrothermal heating (41.1 slpm air vs. 1 slpm nitrogen, respectively)

Figure 3-34. Modeled and Measured Temperatures of Cartridges as a Function of Time for Electrothermal Heating (T1: 1.5 cm, T2: 5.75 cm, T3: 14.25 cm, and T4: 18.5 cm from bottom of cartridges)
Figure 3-35. Modeled and Measured Temperatures of Cartridges as a Function of Time for Heating with Hot Air (T1: 1.5 cm, T2: 5.75 cm, T3: 14.25 cm, and T4: 18.5 cm from bottom of cartridges)

Figure 3-36. Distribution of Thermal Energy: Electrothermal Heating vs. Heating with Hot Air

Electrothermal Heating
(total energy=12.8 kJ)

Heating with Hot Air
(total energy=113.8 kJ)
3.2.2. Mathematical Modeling of Heat and Mass Transfer

Modeling results presented here are based on the mathematical equations described in the section 2.4 with no fitting parameters. Comparisons between modeled and measured power and temperature results for SST desorption of MEK at 500 ppmv and 5,000 ppmv are shown in Figure 3-37. AAEs between measured and modeled cartridge temperatures are 7.4% and 6.6% for SST desorption of MEK at 500 ppmv and 5,000 ppmv, respectively. AAEs between measured and modeled vessel wall temperature are 7.9% and 6.7% for SST desorption of MEK at 500 ppmv and 5,000 ppmv, respectively. AAEs between measured and modeled power are 19.9% and 12% for SST desorption of MEK at 500 ppmv and 5,000 ppmv, respectively.

ESA-R was simulated for run 1 of the screening test (adsorbent: ACFC-20, relative pressure = 0.00169, packing density = 18.3 g/l, nitrogen flow rate = 1 slpm, maximum heating temperature = 300°C, number of cartridges = 2, heating algorithm: constant current) to provide an initial evaluation of the model predictions for a typical set conditions for a regeneration cycle. Comparisons between modeled and measured temperatures are shown in Figure 3-38 and Figure 3-39. AAE values are 7.9% and 2.9% between measured and modeled cartridge temperatures and vessel wall temperatures, respectively. Calculated and measured liquid MEK recoveries are 3.1 g and 2.7 g, respectively for 5.1 g of MEK entering the system. Calculated and measured energy/mass of liquid MEK recovered values are 27,559 J/g and 31,950 J/g, respectively.
Figure 3-37. Comparison of Experimental and Modeling Results for SST Desorption of MEK
Figure 3-38. Modeled and Measured Temperature Profile of Cartridge as a Function of Time for run #1 Screening Experiment

Figure 3-39. Modeled and Measured Temperature Profile of Vessel Wall as a Function of Time for Run #1 Screening Experiment
4. RESEARCH SUMMARY

4.1. Electrothermal-Swing Adsorption with Liquid Recovery

An automated bench-scale adsorption device was designed and used to study effects of select independent engineering parameters on the ability of the system to capture and recover a hazardous air pollutant (HAP, e.g., toluene) from air streams. Experiments were completed in two stages: Stage I consisted of “Screening Experiments” and Stage II consisted of “Central Composite Design experiments.” The screening experiments were used to identify significant factors. Response surfaces for the significant factors were then determined during the second stage of the experiments.

The factors studied during the screening experiments were: type of activated carbon fiber cloth (ACFC) adsorbent, relative pressure of the HAP, packing density of the ACFC, purge gas flow rate, adsorbent regeneration algorithm, and material used for the adsorption vessel, number of adsorbent cartridges, and maximum temperature of adsorbent cartridges during regeneration. Two levels were selected for each factor, which resulted in 20 experiments for the first stage of tests. It was determined during the first stage of the tests that packing density of the adsorbent, regeneration temperature of the adsorbent, and relative pressure of the vapor were significant factors. These factors were studied at five levels in 20 CCD experiments. Analysis of CCD experiments indicated that two cartridges instead of four cartridges should be used per vessel, ACFC-15 instead of ACFC-20 should be used as the adsorbent, and gas flow rate during desorption should be kept at minimum level.

One important improvement is reduction in the amount of power applied per unit mass of ACFC in the vessel. The new value of this energy requirement, 4.7 W/g ACFC represents a reduction of 32.8% over the current value of 7 W/g ACFC. Another important improvement was a scale-up model of the ESA system that was developed by Kaldate (2005) by incorporating the experimental results obtained from this work in order
to optimize the VaPRRS. These results were also used to scale-up this novel technology (Ramirez et al., 2006; Vidal et al., 2006).

4.2. Electrothermal-Swing Adsorption with Steady-State Tracking Desorption

A new method to achieve steady-state tracking (SST) and dynamic-tracking desorption of organic compounds from ACFC was developed and tested with a bench-scale system. ACFC was used to adsorb MEK, acetone, and toluene from air streams. Direct electrothermal heating was then used to desorb the vapor and provide a readily controllable feed stream of that vapor in air at a specified concentration and gas flow rate. The resulting vapor concentration was readily controlled at a user-defined set-point concentration and at 20% of the total gas flow rate that was treated during the adsorption cycle. Low concentration SST desorption with a 500 ppmv set-point concentration was used to provide feed streams that could be fed to a biofilter, while high concentration SST desorption with a 5,000 ppmv set-point concentration was used to provide feed streams that could be fed to an thermal oxidizer. A dynamic set-point concentration which also varied between 250 ppmv and 5,000 ppmv, while also allowing the flow rate of the carrier gas to change by 100%. Such dynamic conditions were used to demonstrate the flexibility of the system in terms of the quick response of the outlet vapor concentration to the variation in set-point concentration and flow rate of the carrier gas during regeneration.

The measured concentration during the low concentration SST desorption test was 496±3 ppmv (mean ± standard deviation) with an average absolute error (AAE) value between the set-point concentration and the measured concentration of 0.94%. The average measured concentration during the high concentration SST desorption was 4,962±32 ppmv with an AAE of 0.8%. Results from the dynamic SST outlet concentration tests at two air flow rates demonstrate that the system is very responsive at controlling the outlet concentration of MEK based on the set-point concentrations with an AAE value for the measured and set-point concentrations of 2.8%.
Concomitant adsorption and desorption (CAD) in dry and humid air streams was tested to investigate the impact of variable inlet organic vapor concentrations (e.g., MEK), and high inlet relative humidity conditions (multi-component inlet gas stream) on the ability of ESA to provide a constant outlet organic vapor concentration. AAE values between the measured outlet and the set-point MEK concentrations were very encouraging at 0.4% (dry air) and 0.3% (humid air). The small AAE values for dry and humid inlet gas streams reflects the ability of the CAD systems to readily control the outlet organic vapor concentration for dry and humid inlet gas streams.

These results demonstrate for first time that SST, dynamic-tracking, and CAD of organic vapor can be readily achieved with ESA technology to provide a gas stream with a readily controlled gas flow rate and organic vapor concentration, even if there is a rapid change in total gas flow rate. The resulting gas stream could be tailored for further processing in a manufacturing process, or treated at a high concentration by an oxidizer or at a low concentration by a biofilter. These results were also used to scale-up this novel technology (Emamipour et al., 2008a).

4.3. CFD Simulations of Fluid Flow and Heat Transfer

Computational fluid dynamic simulations were used to model the three-dimensional (3-D) pressure drop and velocity patterns in an adsorption vessel that contains four annular cartridges of ACFC. Pressure drop and velocity patterns are uniform along 80% of the cartridges. The change in flow patterns over the remaining 20% of the cartridge is due to the brackets that support the cartridges in the adsorption vessel. More than 99% of the pressure drop across the vessel is due to the ACFC cartridges. The remaining pressure drop was caused by gas flowing through the inlet and outlet of the vessel and through the vessel’s interior (excluding the cartridges). These results demonstrate that pressure drop and velocity patterns can be simulated in 1-D or 2-D space, instead of the more complicated 3-D space, for an adsorption vessel that contains four cartridges of ACFC.

2-D simulation of fluid flow through a pleated ACFC filter was tested as another configuration of the adsorbent. It was demonstrated that similar to cylindrical cartridges,
the pressure drop caused by the ACFC cloth is more than 99% of the total pressure drop across the entire assembly. It was shown that gas velocity inside the filter is uniform allowing for another configuration for future generations of ESA.

3-D simulation of heat transfer and fluid flow was performed for electrothermal heating and heating with hot air. It was demonstrated that only 13% of consumed energy is being used for heating of cartridges in hot air heating compare to 78% for electrothermal heating.

4.4. Mathematical Modeling

A mathematical model to simulate ESA was developed and evaluated with experimental data from a bench-scale system. The model consists of: a) material balances for organic vapors in the adsorption vessel and b) energy balances for the adsorbent, carrier gas, vapor, and fittings. Simulated temperature of the cartridges, temperature of vessel wall, and power applied during the regeneration cycles were compared to the experimental data. Model predictions are very encouraging with AAE less than 8% for temperature and less than 20% for power.

4.5. Future Research

Further optimization and development of VaPRRS at the full scale should be completed based on experimental results from this research and optimization models developed by Kaldate (2005). Future designs can make VaPRRS more efficient with respect to lower energy consumption and higher liquid recovery at more competitive cost when compared to existing technologies such as temperature swing adsorption using steam or hot inert gas. This research was focused on the cylindrical cartridges located inside the cylindrical vessels. Other designs of VaPRRS such as pleated filters and the use of low mass/thermal conductivity frames for the ACFC should be evaluated and compared to the current version of VaPRRS to make VaPRRS more energy efficient and therefore more cost-effective technology. New full-scale designs can also account for variability in operating parameters that are experienced in the field that are not accounted for in the laboratory (e.g., very complex multi-component gas mixtures that exist with
coating operations). Further research should also occur with the capture and recovery of multi-component organic vapors and gases from gas streams to make VaPRRS even more efficient. Another area of future research is to develop ACFCs with more selectivity between the gaseous contaminant and other constituents in the carrier gas. For example, treatment of humid gas streams is more costly because water vapor is a competitive adsorbate, especially when relative humidity is more than 40%. Design of hydrophobic ACFCs can be achieved by decreasing the density of oxygen functional groups on the ACFCs. These new materials should be tested in actual ESA systems while treating realistic gas streams.

ESA-SST and ESA-CAD systems were successfully tested on a proof of concept basis in the laboratory with this research but without optimization. Further enhancement of the performance of these systems should occur. The relative difference between the set-point and the measured concentration can be decreased by more careful tuning of the proportional integral derivative control parameters. It was demonstrated that the purge gas stream consumes the majority of energy. Using a heat exchanger between the inlet and outlet gas streams will improve the thermal efficiency of these systems. This will also decrease the carrier gas temperature making the stream more suitable for biofiltration. Similar to VaPRRS, further research on capture of multi-component organic vapor gas streams will help the design of even more efficient SST and CAD systems. It would be enlightening to assess the performance of a biofilter and an oxidizer by using the SST and CAD systems upstream of a biofilter or an oxidizer. Overall optimization of a SST or a CAD system integrated with a secondary air pollution control device needs to be performed in to minimize the overall system cost while maximizing the performance of the system.

CFD simulations provided qualitative description of fluid flow and heat transfer within an adsorption vessel. These successful simulations were encouraging and enhanced the understanding of flow patterns and heat transfer for ESA. However, no mass transfer was included in the CFD simulations. This work can be extended to the simulation of simultaneous momentum, heat, and mass transfer. Both CFD simulations
and 1-D modeling of heat and mass transfer that were developed for cylindrical cartridges in a cylindrical vessel can be extended to a broader range of configurations (e.g., pleated filters in a rectangular vessel). Such simulations will provide very valuable information as part of optimizing the system.

ESA-VaPRRS/SST/CAD have the potential to be used for both indoor and outdoor air quality applications at relatively low cost. ESA can be tested for typical of air pollutant mixtures encountered in indoor air such as those that contain 2-propanol, 2-butoxyethanol, camphene, and terpineol. Evaluations should occur over extended periods of at least several months by varying the air’s relative humidity and VOC concentrations. Cost should also be developed to estimate the costs of installing and operating commercial ESA devices for use in indoor environments.
5. REFERENCES


USEPA (2007a) www.epa.gov/tri/


Yu et al., (2002)
6. NOMENCLATURE

A \quad \text{Specific surface of adsorbent}

A_c \quad \text{Outer surface area of cartridges}

A_w \quad \text{Internal surface area of vessel wall}

C \quad \text{Inertial resistance factor}

C_A \quad \text{Concentration of adsorbate in gas phase}

C_A^* \quad \text{Equilibrium concentration of adsorbate in gas phase}

C_{A,in} \quad \text{Concentration of adsorbate in inlet gas stream}

C_A^i \quad \text{Initial concentration of adsorbate in the gas phase}

C_{p,g} \quad \text{Heat capacity of gas}

C_{p,l} \quad \text{Heat capacity of liquid adsorbate}

C_{p,s} \quad \text{Heat capacity of adsorbent}

C_{p,w} \quad \text{Heat capacity of vessel wall}

F_{c-w} \quad \text{Radiation shape factor}

h_1 \quad \text{Heat transfer coefficient- inner surface of cartridges}

h_2 \quad \text{Heat transfer coefficient- outer surface of cartridges}

h_3 \quad \text{Heat transfer coefficient- inner surface of vessel wall}

h_4 \quad \text{Heat transfer coefficient- outer surface of}
\( h_b \) 
Heat transfer coefficient

\( k_c^{\text{eff}} \) 
Effective thermal conductivity of adsorbent

\( k_g^{\text{eff}} \) 
Effective thermal conductivity of gas in bed

\( k_m \) 
Mass transfer coefficient

\( k_w \) 
Thermal conductivity of vessel wall

\( L \) 
Length of ACFC cartridge

\( M_A \) 
Molecular weight of adsorbate

\( M \) 
Number of cartridges in electrical series

\( m_5 \) 
Amount of adsorbed adsorbate in the ACFC when outlet concentration has reached 5% of inlet concentration

\( m_{\text{sat}} \) 
Mass of the organic vapor adsorbed at saturation

\( m_{a,\text{eq}} \) 
Equilibrium loading of MEK that existed at the end of the regeneration cycle

\( m_{a_i} \) 
Amount of initially adsorbed MEK during the preceding adsorption cycle

\( m_{a_i,\text{eq}} \) 
Initial equilibrium loading of MEK from the previous adsorption cycle

\( M_{\text{MEK}} \) 
Molecular weight of MEK

\( M_{\text{MEK}} \) 
Molecular weight of MEK

\( MW_A \) 
Molecular weight of adsorbate

\( N \) 
Number of cartridges in each bank

\( n_l \) 
Number of layers of cloth

\( n_e \) 
Number of separate electrical circuit
\( n_p \) \hspace{1cm} \text{Number of parallel circuits in each separate circuit}

\( n_s \) \hspace{1cm} \text{Number of cartridges series for each parallel circuit}

\( P \) \hspace{1cm} \text{Pressure}

\( P_i \) \hspace{1cm} \text{Pressure at the inner surface of ACFC cartridge}

\( P^o \) \hspace{1cm} \text{Standard pressure}

\( P^o \) \hspace{1cm} \text{Standard pressure}

\( P_o \) \hspace{1cm} \text{Pressure at the outer surface of ACFC cartridge}

\( Q \) \hspace{1cm} \text{Actual gas flow rate}

\( Q \) \hspace{1cm} \text{Concentration of adsorbate in solid phase}

\( Q \) \hspace{1cm} \text{Actual gas flow rate}

\( q^i \) \hspace{1cm} \text{Initial concentration of adsorbate in solid phase}

\( q_{\text{sat}} \) \hspace{1cm} \text{Saturation adsorption capacity of cloth}

\( Q^o \) \hspace{1cm} \text{Gas flow rate at standard conditions}

\( Q^o_{\text{reg}} \) \hspace{1cm} \text{Flow rate of air during the regeneration cycle at STP}

\( R \) \hspace{1cm} \text{Ideal gas law constant}

\( R \) \hspace{1cm} \text{Radial coordinate}

\( R_g \) \hspace{1cm} \text{Ideal gas law constant}

\( r_i \) \hspace{1cm} \text{Inner radius of ACFC cartridge}

\( r_{i,c} \) \hspace{1cm} \text{Inner radius of cartridges}

\( r_o \) \hspace{1cm} \text{Outer radius of ACFC cartridge}

\( r_{o,c} \) \hspace{1cm} \text{Outer radius of cartridges}
T  
Time

T  
Temperature

T_{amb}  
Ambient temperature

T_{b1}  
Average gas temperature in inlet tubes

T_{b2}  
Average gas temperature in vessel

T_c  
Temperature of solid

T_{c, i}  
Initial adsorbent temperature

T_g  
Temperature of gas

T_{g, in}  
Inlet gas temperature

T_{g, i}  
Initial gas temperature

T_{i}  
Initial gas temperature in vessel

T_{b1}  
Initial gas temperature in inlet tubes

T_{b2}  
Initial gas temperature in vessel

T^o  
Standard temperature

T^o  
Standard temperature

t_5  
time required to achieve 5% breakthrough

\text{t}_{50}  
time required to achieve 50% breakthrough

t_{reg}  
Total regeneration time

T_w  
Temperature of vessel wall

t_{ACFC}  
Thickness of ACFC cloth

\text{t}_{ads}  
Adsorption cycle time

U  
Velocity component

V  
Velocity vector, m/s

V_{b1}  
Volume of inlet tubes

V_{b2}  
Volume of vessel excluding cartridges and inlet tubes
\( w_o \)  
Total micropore volume

\( X \)  
Cartesian coordinate vector

\( y_{ou} \)  
Mole fraction of MEK of the outlet gas stream

\( Z \)  
Vertical coordinate

\( \dot{q} \)  
Heat generation rate

\( \hat{h} \)  
Enthalpy

\( u' \)  
Fluctuating component of the velocity

\( \Delta H_{ads} \)  
Heat of adsorption

\( \Delta t \)  
Time interval

\( \alpha \)  
Permeability

\( \delta \)  
Kronecker’s delta

\( \delta t \)  
Time interval

\( \varepsilon \)  
Inter fiber porosity of adsorbent

\( \varepsilon_c \)  
Emissivity of adsorbent

\( \varepsilon_w \)  
Emissivity of vessel wall

\( \kappa \)  
DQSAR parameter

\( \mu \)  
Viscosity

\( \rho \)  
Density

\( \rho_b \)  
Density of the cartridges

\( \rho_e \)  
Electrical resistivity of cloth

\( \rho_{cvlp} \)  
Envelope density of ACFC fibers

\( \rho_f \)  
Density of ACFC fibers

\( \rho_g \)  
Gas density
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho_{LA} )</td>
<td>Density of liquid adsorbate</td>
</tr>
<tr>
<td>( \rho^g )</td>
<td>Gas density at standard conditions</td>
</tr>
<tr>
<td>( \rho_w )</td>
<td>Density of vessel wall</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>Stefan-Boltzmann's constant</td>
</tr>
<tr>
<td>( \zeta )</td>
<td>Factor for the adsorbate remaining after regeneration</td>
</tr>
</tbody>
</table>
7. CURRICULUM VITAE

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Education

<table>
<thead>
<tr>
<th>Degree</th>
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<th>Date Awarded</th>
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<tr>
<td>Ph.D.</td>
<td>Environmental Engineering</td>
<td>University of Illinois, UI</td>
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<tr>
<td>M.S.</td>
<td>Chemical Engineering</td>
<td>Shiraz University, Iran</td>
<td>1997</td>
</tr>
<tr>
<td>B.S.</td>
<td>Chemical Engineering</td>
<td>Shiraz University, Iran</td>
<td>1994</td>
</tr>
</tbody>
</table>

Professional Experiences

Research Assistant, Civil & Environmental Engineering (CEE) Department, UI, 2002 - present.
Teaching Assistant, Chemical Engineering Department, Shiraz University, 1995 – 2000.
Research Assistant, Chemical Engineering Department, Shiraz University, 1992 – 2000.

Awards and Honors

Travel Award from Ministry of Science, Research & Technology of Iran, 2001.
Ranked 1th in the Nation-Wide Chemical Engineering Examination, 1994.

Professional Memberships

Air & Waste Management Association (A&WMA, member), 2003 – present.
American Society of Chemical Engineers (AIChE, member), 2007 – present.
Computer Skills
Software packages: Comsol Multiphysics, Fluent, Gambit, Tecplot, ANSYS, FlexPDE, Labview, Microsoft Word, Excel, and PowerPoint.
Programming languages: C, C++, FORTRAN, MATLAB.

Research Experience
Design, build, and experimental study of bench-scale Electrothermal Swing Adsorption (ESA) system.
Assisting in the design of full-scale ESA systems.
Mathematical modeling of heat and mass transfer in ESA.
Simulation of fluid flow in ESA by using FLUENT software package.
Design and build bench-scale distillation column, evaporator, and mobile bed absorber.
Assisting in the design of a plant for production of table salt by washing method.

Management of Research Group Members
Mentored four undergraduate research assistants to develop meaningful research experience: Zachary Schuste, Kevin Kyrias-Gann (building experimental setup, lab maintenance and supplies), Andrew Riley (lab maintenance and supplies), and Dave Johnsen (calculation of adsorption capacity of activated carbon fiber clothes for organic vapors).

Publications
Peer Reviewed Journal Publications:

Conference Proceedings:


