Original citation:

Permanent WRAP URL:
http://wrap.warwick.ac.uk/79785

Copyright and reuse:
The Warwick Research Archive Portal (WRAP) makes this work by researchers of the University of Warwick available open access under the following conditions. Copyright © and all moral rights to the version of the paper presented here belong to the individual author(s) and/or other copyright owners. To the extent reasonable and practicable the material made available in WRAP has been checked for eligibility before being made available.

Copies of full items can be used for personal research or study, educational, or not-for-profit purposes without prior permission or charge. Provided that the authors, title and full bibliographic details are credited, a hyperlink and/or URL is given for the original metadata page and the content is not changed in any way.

A note on versions:
The version presented here is a working paper or pre-print that may be later published elsewhere. If a published version is known of, the above WRAP url will contain details on finding it.

For more information, please contact the WRAP Team at: wrap@warwick.ac.uk
ABSTRACT: In the prospect of manufacturing specific activated carbon adsorbent, a research work is carried out with the objective of screening a large number adsorbent models (more than 60,000) and identifying suitable ones with optimum characteristics for three applications: Ice marking ($T_C=35^\circ C$, $T_E=-5^\circ C$), Air conditioning ($T_C=35^\circ C$, $T_E=15^\circ C$) and Heat pump ($T_C=40^\circ C$, $T_E=5^\circ C$). For each application, the driving temperature will range from 65$^\circ C$ to 200$^\circ C$. Overall, the preliminary simulation results show that for each adsorbent model with each application, the refrigerant uptake variation has an optimum.

INTRODUCTION

Many solid adsorbents on the market are often mainly specified and manufactured for industrial processes like gas separation, cracking and storage, gas or air filtration and drinking water treatments. Those manufacturing specifications are mainly BET surface area ($m^2/g$), specific volume ($cm^3/g$), particle size median ($\mu m$) or micro-pores size distribution, grain size (mm x mm) or mesh size (Sieve Number x mm) and bulk density (kg/m$^3$). Currently, to manufacture reactors for thermal compressors dedicated to heat pump and refrigeration applications, the adsorbents selected will not necessarily meet optimum specifications for the purpose. The proposed work is an attempt to elaborate a tool that is designed to identify optimum manufacturing specifications of adsorbent-adsorbate pair for heat pump and refrigeration applications. For that purpose and with the thermal compressor driving temperatures ranging from 65$^\circ C$ to 200$^\circ C$, three specific applications are under scrutiny: Ice making ($T_{Evaporation}=-5^\circ C$, $T_{Condensation}=35^\circ C$), Air Conditioning ($T_{Evaporation}=10^\circ C$, $T_{Condensation}=35^\circ C$) and Heat Pump ($T_{Evaporation}=5^\circ C$, $T_{Condensation}=40^\circ C$).

METHODOLOGY

The methodology is mainly based on a modified form of the Dubinin-Astakhov (D-A) equation \[1, 2\].

$$x = x_o \exp \left[ -k \left( \frac{T}{T_{sat}} - 1 \right)^n \right]$$

(1)

Where $x$ is the refrigerant concentration (kg refrigerant/kg adsorbent); $T$ is the carbon temperature (K); $x_o$ is the refrigerant concentration under saturation conditions (kg refrigerant/kg adsorbent); $T_{sat}$ is the saturation temperature corresponding to the gas pressure (K); $k$ is defined as the energetic affinity characteristic of adsorbent-refrigerant pair and $n$ is the characteristic of adsorbent micro-pores size distributions. The method consists of scanning all combinations of $x_o$ (0.1 to 1 with 0.05 as increment) by $k$ (1 to 50 with 1 as increment) and by $n$ (1 to 6 with 0.1 as increment), and identifying the optimum value of a key performance indicator like the refrigerant uptake variation $\Delta x$, COP, specific cooling or heating for specific application and operating conditions. For this initial study, the uptake swing ($\Delta x$) is used as figure of merit. From the identified values of $x_o$, $k$ and $n$, the main objective will then be to translate them into some form of adsorbent manufacturing specifications. The full algorithm diagram of the proposed method is shown in Figure 1.
The current paper gives an overview of preliminary simulation results. Figure 2 shows an example of refrigerant concentration variation for all possible operating conditions with $x_o=0.40 \text{ kg refrigerant/kg adsorbent}$ (for illustration $n$ values with increment of 1); for this same value of $x_o$, optima are identified at specific values of both $k$ and $n$ (illustration in Figure 3 for Ice Making application with a driving temperature of 100°C). Furthermore, for each value of $k$, there is an optimum at a given value of $n$. Since adsorbed refrigerant is always assumed to be in a liquid form located in the adsorbent micro-pores, the maximum uptake of refrigerant by the adsorbent ($x_o$) is calculated from the specific volume of micro-pores ($v_s$) and the refrigerant liquid density at normal pressure condition (atmospheric pressure) ($\rho_L$):

$$x_o = \rho_L v_s \Rightarrow v_s = \frac{x_o}{\rho_L}$$

(2)

Figure 4 shows the variation of adsorbent specific volume with refrigerant liquid density and for different values of $x_o$. For refrigerant liquid with more than 600 kg/m$^3$ in density, the first indication is that the adsorbent specific volume must not exceed 0.80 cm$^3$/g.
Figure 2: An example of refrigerant concentration variation for all possible operating conditions.

Figure 3: Example uptake swing ($\Delta x$) variation function of $n$ and $k$ parameters for Ice Making application with driving temperature of 100°C.
Figure 4: Adsorbent specific volume vs. refrigerant liquid density for different values of $x_o$. (The density of Carbon Dioxide is estimated to 640 kg/m$^3$ [3, 4]).

CONCLUSIONS

The preliminary simulation results show that for each adsorbent model with each application, the refrigerant uptake variation has an optimum. As illustration for ice making application with a driving temperature of 100°C, $x_o=0.40$ kg/kg, $k=3$ and $n=1.4$ is an example of best model based on uptake swing ($\Delta x$) as figure of merit. For this example with the selection of Ammonia (R717) as refrigerant, the adsorbent specific volume will then be 0.30 cm$^3$/g.

FUTURE WORK

Future work will include both heating and cooling capacities and COP as key performance indicators for optimization with additional manufacturing specifications of adsorbent (BET surface area, particle size median or micro-pores size).

ACKNOWLEDGEMENTS

This is a follow up work from initial project supported by EPSRC (UK) and Chemviron Carbons Ltd (UK) under the grant EP/J000876/1

References: