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Psychrometric-like charts for the energy analysis of VOC recovery processes

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Abstract

Psychrometric-like charts for the energy analysis of VOC removal or recovery by means of combined adsorption and condensation were developed. These charts make use of conventional psychrometric parameters: dry-bulb temperature, specific mass content—or alternately mole fraction—, degree of saturation (relative "humidity"), enthalpy, etc., for toluene-nitrogen mixtures. In addition, they include information on the adsorption equilibrium, and particularly the adsorbed-phase enthalpy, in order to characterise the adsorbers behaviour. The graphical representations of unitary operations occurring in VOC treatment processes are presented: VOC condensation on a cool coil, adsorption or regeneration of an adsorber. This methodology is applied to a case study based on an indirectly heated and cooled adsorber and a heat pump. A proper design of this integrated process allows to use half of the heat available at the heat pump condenser, which is usually wasted.

Keywords: VOC recovery; Psychrometric chart; TSA (temperature swing adsorption); Condensation

1. Introduction

Among the various VOC removal or recovery processes, adsorption (often TSA processes) and refrigeration (condensation) are usually not competitors, but rather applicable for relatively different operating conditions. For instance, Le Cloirec [1] recommends the use of adsorption for VOC concentration ranging from 0.5 to 5 $g \cdot m^{-3}$ with a flow rate between 100 and 50 000 $m^3 \cdot h^{-1}$, while condensation should be used for higher concentrations (20–100 $g \cdot m^{-3}$) and for a wider flow rates range (50–100 000 $m^3 \cdot h^{-1}$). This is why these methods can be operated successively following a combined process. Moreover, TSA processes imply a heat consumption, but their performances can be noticeably enhanced if the adsorber is cooled during the adsorption step, so as to limit the adsorption-driven temperature overshoot [2,3].

Keeping in mind that refrigeration plants reject heat at their condenser—a heat which is often wasted—, it has sometimes been proposed [4,5] to develop combined processes aiming to find out the best use of energy for VOC removal or recovery, with the best possible process performances.

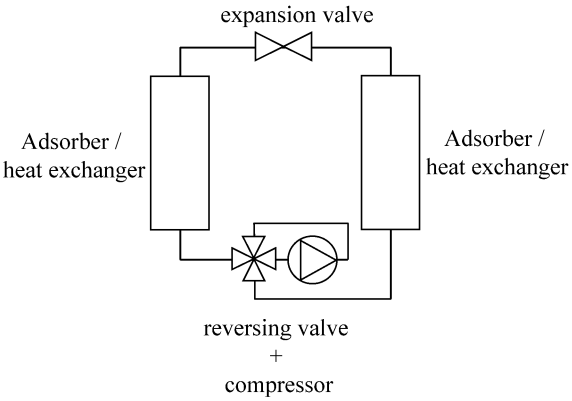

Fig. 1. Architecture of a directly-combined system (one adsorber/exchanger under regeneration/condensation and one under adsorption/evaporation).

A first combined process (Fig. 1) consists in using simultaneously two adsorbers, one in adsorption and the other in regeneration, but the former is cooled down by the evaporator while the latter is heated up by the condenser of a heat-

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Nomenclature

C	gas phase concentration	$\text{kg}\cdot\text{m}^{-3}$
c_p	heat capacity	$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
E	efficiency	
h	enthalpy	$\text{J}\cdot\text{kg}^{-1}$
K	Toth equation parameter	Pa^t
m	mass of gaseous species	kg
M	mass of solid species	kg
$\overline{M}$	molar mass	$\text{kg}\cdot\text{mol}^{-1}$
n	molar adsorbed phase concentration	$\text{mol}\cdot\text{kg}^{-1}$
P	pressure	Pa
q	adsorbed phase concentration in weight	$\text{kg}\cdot\text{kg}^{-1}$
Q	heat	J
Q	Toth equation parameter	$\text{J}\cdot\text{mol}^{-1}$
r	mass gas constant	$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
R	universal gas constant, $= 8.314\ \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	
t	Toth equation parameter	
T	temperature	K
V	volume	m^3
w	specific mass content	$\text{kg}\cdot\text{kg}^{-1}$
y	gas mole fraction	

Greek symbols

α	Toth equation parameter	
ΔH	adsorption heat	$\text{J}\cdot\text{mol}^{-1}$
Δh_{lv}	latent heat of vaporisation	$\text{J}\cdot\text{kg}^{-1}$
Δw	variation of specific mass content	$\text{kg}\cdot\text{kg}^{-1}$
ε	degree of saturation	%
χ	Toth equation parameter	K^{-1}

Subscripts

AC	activated carbon
ads	adsorption
cool	cooling
des	desorption
dew	dew point
metal	metallic parts
N_2	nitrogen
tol	toluene
sat	saturation

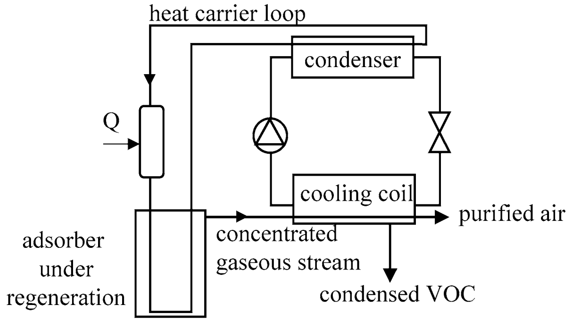

Fig. 2. Adsorption followed by VOC condensation.

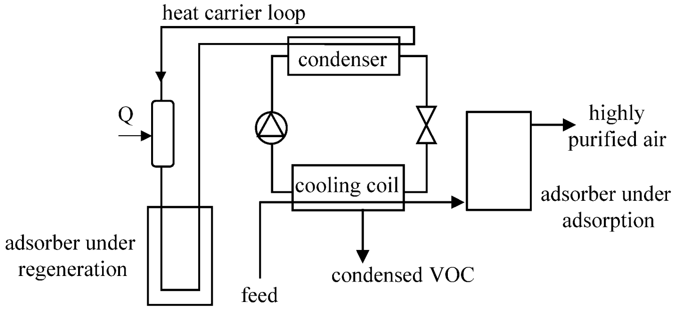

Fig. 3. VOC condensation followed by an adsorption step.

pump. When the adsorbing adsorber is saturated and the other is regenerated, the heat pump cycle is reversed. This process architecture does not allow recovering a condensed stream of VOC: it allows the recovery of a gaseous stream, sometimes enriched with respect to the feed. In addition, this architecture cannot be recommended if the needs in refrigerating and heating power are of the same order of magnitude: they approximately differ from the mechanical power supplied to the heat pump, which is typically 1/3 of the cooling capacity (i.e. 1/4 of the heating capacity, assuming that the COP—COefficient of Performance—is close to 3). Lastly, for a proper operation, the time for both steps (adsorption and regeneration) should be close enough to each other.

Another possibility of combined system lies in the successive use of condensation and adsorption, in their best operating conditions. For instance, with a less than 10 $\text{g}\cdot\text{m}^{-3}$ feed, an adsorption step should be used first. Once the adsorber is saturated, it should be regenerated with the indirect heating and cooling process developed by Bonjour et al. [6] so as to reach a more concentrated stream (between 10 to 100 $\text{g}\cdot\text{m}^{-3}$) that can hence be easily condensed on a cooling coil. This system (Fig. 2) should use the heat available at the heat-pump condenser to regenerate a second adsorber. If this heat is not sufficient, a supplementary heat should be provided to that integrated process. An alternative to this architecture is depicted on Fig. 3: in this case, the adsorption follows the condensation.

A proper design of such integrated processes requires the use of engineering tools able to represent both the heat and mass transfers in the various devices constituting the process. The complex phenomena involved in such processes can be investigated by means of numerical simulations, each model being correctly connected to the others. The complexity of this task makes it inappropriate in a first approach. On the contrary, oversimplified approaches might lead to inaccurate designs. This is the reason why the present article aims to develop a new tool allowing to analyse integrated process with a reasonable tradeoff between complexity and accuracy: psychrometric-like chart for VOC-nitrogen mixtures in the presence of an adsorbent. We will first see in the following how to draw such charts. Then, from an analogy with moist-air operations in the airconditioning field, we will discover how to use these charts for evaluating the performance of a combined TSA-condensation process.

According to Shallcross and Low [7], psychrometry is "the study of systems in which one or more vapour components condense while the other components remain gaseous". These authors presented some psychrometric charts for various VOC-nitrogen pairs, among which toluene and nitrogen. The choice of the state equations (Virial formulation, excess variables in order to take into account the non-ideality of such mixtures) was also discussed by Shallcross [8]. Recently, this author extended the development of such psychrometric-like charts to various ketones-dry air systems [9]. These charts were however not used for describing unitary operations but rather to analyse the thermodynamic equilibrium. Here, we intend to use simpler state equations, but also to propose a practical example of use of the chart that will include information concerning the adsorption equilibrium. We will also compare the advantages and drawbacks of molar and mass-based diagrams.

2. Psychrometric-like chart for VOC-nitrogen mixtures in the presence of an adsorbent

2.1. Gaseous mixture properties

Assuming ideal gas law for nitrogen (denoted N_2) and toluene (denoted tol), the total pressure P of a nitrogen-toluene mixture is:

$$P = P_{N_2} + P_{\text{tol}}$$
$$\text{with } P_{N_2} V = m_{N_2} r_{N_2} T \text{ and } P_{\text{tol}} V = m_{\text{tol}} r_{\text{tol}} T \tag{1}$$

Because of the molecular weights ($\overline{M}_{N_2} = 28$ g·mol^{-1} and $\overline{M}_{\text{tol}} = 92$ g·mol^{-1}) and universal gas constant, the numerical values for the mass constants are $r_{N_2} = R/\overline{M}_{N_2} = 286.7$ J·kg^{-1}·K^{-1} and $r_{\text{tol}} = 90.4$ J·kg^{-1}·K^{-1}.

Now reasoning with a unitary mass of nitrogen ($m_{N_2} = 1$ kg) and a corresponding mass of toluene (w, in kg of toluene per kg of nitrogen, which is called "specific mass content"), Eq. (1) yields:

$$w = 3.172 \frac{P_{\text{tol}}}{P - P_{\text{tol}}} \tag{2}$$

The specific mass can be accompanied by the mole fraction (y) or the gas-phase concentration (C in kg·m^{-3}):

$$y_{\text{tol}} = \frac{w/\overline{M}_{\text{tol}}}{w/\overline{M}_{\text{tol}} + 1/\overline{M}_{N_2}} \quad \text{and} \quad C_{\text{tol}} = \frac{w \cdot P}{T \cdot (r_{N_2} + w \cdot r_{\text{tol}})} \tag{3}$$

The saturation degree (equivalent to moist air "relative humidity") is:

$$\varepsilon = 100 \times \frac{P_{\text{tol}}}{P_{\text{sat}}} \tag{4}$$

where P_{sat} is the saturation pressure given by an appropriate correlation, namely that given by Wagner (cited by Perry [10]).

From the saturation degree, the dew-point temperature is defined as the temperature at which the toluene present in a slowly-cooled mixture starts to condense. In other words, at this temperature, $\varepsilon = 100\%$ and hence $P_{\text{tol}} = P_{\text{sat}}(T_{\text{dew}})$.

In order to perform energy balances, the specific enthalpy of the ideal gases mixture (in kJ·kg$_{N_2}^{-1}$) is written as the sum of the enthalpy of both components:

$$h = c_{p,N_2} \cdot T_{^\circ\text{C}} + w \cdot (\Delta h_{\text{lv}} + c_{p,\text{tol}} \cdot T_{^\circ\text{C}}) \tag{5}$$

This formulation reflects the assumptions that the heat capacities of the components (c_p) and the latent heat of vaporization (Δh_{lv}) of the toluene are constant. In addition, the enthalpies are given with a reference being 0 at $T = 0\,^\circ\text{C}$ for gaseous nitrogen and saturated liquid toluene. Numerically, the values used in the following are: $c_{p,N_2} = 1.04$ kJ·kg^{-1}·K^{-1}, $c_{p,\text{tol}} = 1.141$ kJ·kg^{-1}·K^{-1} and $\Delta h_{\text{lv}} = 363.66$ kJ·kg^{-1}. For a better accuracy, a temperature-dependent formulation for the heat capacities and latent heat of vaporization might have been chosen. However, for the present range of temperatures, the heat capacity of nitrogen variation remains limited. Moreover, the toluene heat capacity increases while its latent heat of vaporization decreases with increasing the temperature, as can be checked from the correlations proposed by Shallcross [8]. From these trends, the difference between enthalpies values calculated from the constant-properties formulation and the temperature-dependent formulation is limited to a few percents, which is covered over by the graphical error when using the chart.

Contrary to the moist air chart, the wet-bulb temperatures will not be defined, because they are not useful in the following. In addition, as stated by Shallcross and Low [7], and for the same reason as in moist air, wet-bulb isotherms and gas-phase isenthalps are very close the one to the other.

2.2. Adsorbed-phase enthalpy

A last information is given on the psychrometric charts: the adsorbed-phase enthalpy in kJ·kg^{-1} of adsorbent. It should be emphasized that, contrary to the previously defined parameters, this variable is specific to the adsorbent-adsorbate pair and not to the equilibrium between gaseous and liquid species. For a unitary mass of adsorbent, this enthalpy is written:

$$h_{\text{ads}} = q_{(P_{\text{tol}},T)} \cdot \bigl(\Delta h_{\text{lv}} + c_{p,\text{tol}} \cdot T_{^\circ\text{C}} - |\Delta H|\bigr) \tag{6}$$

where $q_{(P_{\text{tol}},T)}$, in kg·kg^{-1} of adsorbent, represents the amount of toluene adsorbed under the pressure P_{tol} and the temperature T (i.e. equilibrium adsorption isotherm) and ΔH is the isosteric heat of adsorption. This equation means that the enthalpy of a given amount of adsorbed toluene is the enthalpy of the same amount of gaseous toluene ($h_{\text{tol}} = \Delta h_{\text{lv}} + c_{p,\text{tol}} \cdot T_{^\circ\text{C}}$, cf. Eq. (5)) minus the heat of adsorption involved in the adsorption of the toluene.

In the present charts, we use data given by Saysset [11] for the adsorption of toluene on Ambersorb™ 572. Saysset gives a molar Toth equation for the isotherms:

$$n = n_{\text{sat}} \cdot P/\bigl(K + P^t\bigr)^{1/t} \tag{7}$$

with

$$t = t_0 + \alpha(1 - T_0/T)$$
$$n_{\text{sat}} = n_{0,\text{sat}}\bigl(1 - \chi(T - T_0)\bigr)$$
$$K = K_0 \cdot \exp\bigl(Q/(RT)\bigr) \tag{8}$$

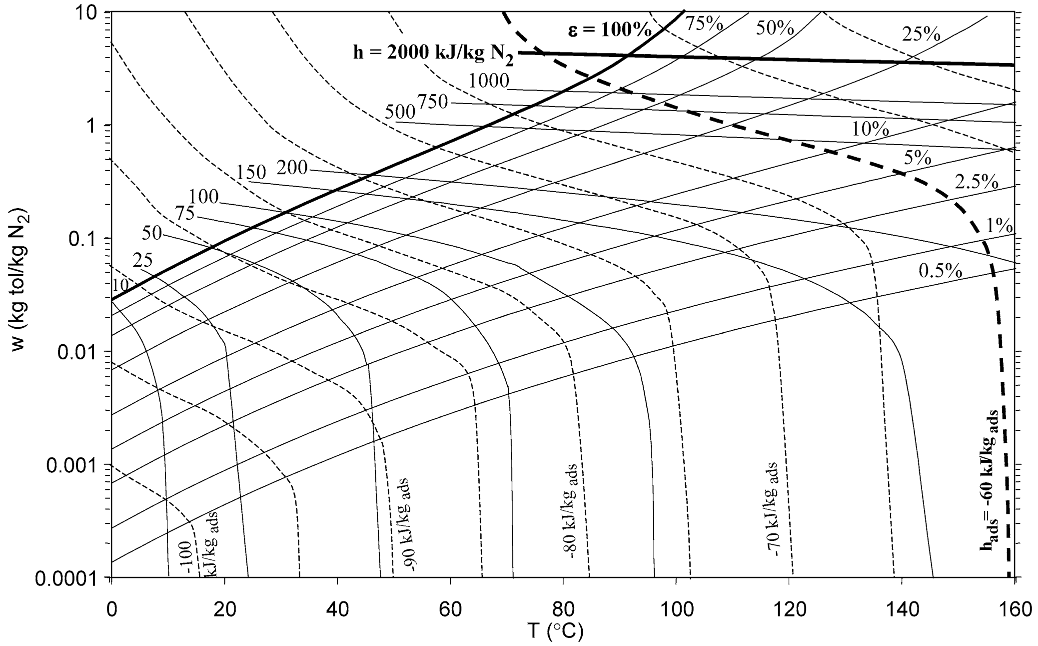

Fig. 4. Semi-logarithmic psychrometric chart for the nitrogen/toluene mixture ($P = 101325$ Pa). Dashed lines: adsorbed-phase isenthalps. The lines of constant enthalpy $h_{\text{ads}} = -60\ \text{kJ}\cdot\text{kg}_{\text{ads}}^{-1}$ and $h = 2000\ \text{kJ}\cdot\text{kg}_{\text{N}_2}^{-1}$ and of constant $\varepsilon = 100\%$ are drawn in bold in order to make easier the identification of their curve family.

Table 1
Toth equation parameters for the adsorption isotherms of toluene on activated carbon Ambersorb™572 [11]

$n_{0,\text{sat}}$ [mol·kg$_{\text{ads}}^{-1}$]	χ [K^{-1}]	K_0 [Pa^t]	Q [J·mol^{-1}]	t_0	α
5.896	-1.12×10^{-3}	40.2	-14.85×10^3	0.149	0.084

The Toth parameters ($n_{0,\text{sat}}$, χ, K_0, Q, t_0 and α) are given in Table 1, with a reference temperature $T_0 = 353$ K. Lastly, Saysset [11] also gives experimental values for the adsorption heat fitted linearly with the adsorbed amount: $\Delta H = -10.15 \times n + 99$, where n is in mol·kg^{-1} of adsorbent and ΔH in kJ·mol^{-1} of toluene.

2.3. Plotting psychrometric charts

From Eqs. (1)–(5), a first diagram (Fig. 4) is plotted under a semi-logarithmic form for a total operating pressure $P = 101325$ Pa. It gives the specific mass content vs. the temperature with lines of constant degree of saturation, of constant gas-phase enthalpy and of constant adsorbed-phase enthalpy. The lines corresponding to $\varepsilon = 100\%$, $h = 2000\ \text{kJ}\cdot\text{kg}^{-1}$ and $h_{\text{ads}} = -60\ \text{kJ}\cdot\text{kg}^{-1}$ are drawn in bold, for the sake of a better visual identification of each curve family. The adsorbed-phase enthalpy is plotted with a dashed line so as to emphasize that they are specific to the adsorbent. A comparable chart will be used in the following but based on the mole fraction rather than in the specific mass content (cf. Eqs. (2) and (3)) as the ordinates. The chart of Fig. 4 does not "look like" conventional moist-air charts: this is due to the choice of semi-logarithmic scale, which is however helpful because of the large variations in the toluene specific mass content or mole fractions encountered in TSA processes (cf. Section 4). On the contrary, if choosing a conventional scale, the overall shapes of the line is directly comparable to the moist-air chart, as shown by Shallcross [9].

It should be underlined that the molar and mass-based charts give different information, but that both are meaningful. Obviously, a first criterion for choosing the chart is the user's wish to reason in terms of moles or kilograms. But in addition to this criterion, it must be recalled that the molar chart is limited to a unitary mole fraction ($y = 1$). On the contrary, the mass-based chart does not have any upper limit, because the specific mass content may always increases, as long as the temperature increases. Indeed, each line of constant degree of saturation increases asymptotically to an infinite specific toluene mass content when the temperature tends towards the maximum temperature for the considered line. This maximum temperature is the saturation temperature calculated for a pressure equal to the total pressure divided by the degree of saturation:

$$w(T)\Big|_{\substack{\varepsilon=\text{constant}\\ P=\text{constant}}} \to \infty \quad \text{when } T \to T_{\text{sat}}(P/\varepsilon P) \tag{9}$$

Because of this absence of upper limit, a higher graphical accuracy is obtained in the mass-based chart than in the molar chart for high temperatures and high concentrations.

3. Graphical representation of elementary processes

The combined VOC recovery processes evoked in the first section can be viewed as the succession of elementary processes that must be graphically represented in the psychrometric charts. Theses graphical representations are described in the next paragraphs.

Adsorption step. An adsorption process (Fig. 5) aims to split the feed (point A) into two phases, namely the fluids (adsorbed

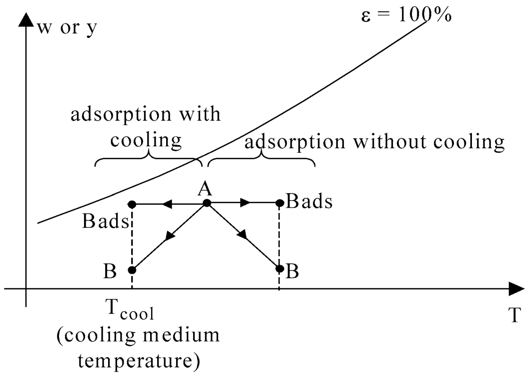

Fig. 5. Graphical representation of an adsorption step with or without cooling.

or interstitial) in the adsorber (point B_{ads}) and the product (i.e. purified nitrogen) represented as point B. The adsorbed-phase is in equilibrium with the surrounding interstitial gas, at the temperature reached in the adsorber at the end of the adsorption step. In the case of an adiabatic adsorber, this temperature is higher than the feed, but in the case of an indirectly cooled adsorber [2,3,6], it is close to the cooling medium temperature. In addition, the interstitial gas mole fraction is imposed by that of the feed, which means that $y_{B\text{ads}} = y_A$. Lastly, the mole fraction or mass-content of point B represent the product purity. In actual processes, the purified effluent concentration slightly varies with time during the adsorption step, but it remains limited to its maximum admissible value and is finally characterised by its time-averaged value (y_B).

Desorption/regeneration step. The regeneration step (Fig. 6) consists in supplying heat and purge gas to the adsorber containing an adsorbed-phase (point C_{ads}) in order to produce two phases: the desorbed-phase (outlet of the adsorber, point D_{des}) and the residual phase that remains inside the adsorber before the next adsorption (point D_{ads}). Similarly to the adsorption step, in actual processes, the outlet stream composition also varies with time during the regeneration step. This is why $y_{D\text{des}}$ represents the time-averaged mole fraction. On the contrary, D_{ads} is not a time-averaged point as it represents a static residual phase.

It is usually convenient to evaluate the energy requirement for this operation. For given masses of adsorbent (M_{AC}), of purge nitrogen (m_{purge}) and of metallic parts of the adsorber (M_{metal}), the energy balance is written:

$$\begin{aligned} Q_{\text{des}} = {} & M_{\text{AC}}(h_{D\text{ads}} - h_{C\text{ads}}) + m_{\text{purge}}(h_{D\text{des}} - h_{\text{purge}}) \\ & + M_{\text{AC}} \cdot c_{p,\text{AC}} \cdot (T_{D\text{ads}} - T_{C\text{ads}}) \\ & + M \cdot c_{p,\text{metal}} \cdot (T_{D\text{ads}} - T_{C\text{ads}}) \end{aligned} \tag{10}$$

In Eq. (10), the first term corresponds to the desorption and sensible heat of the processed toluene, the second to the heat necessary to heat up the purge, and the third and fourth to the sensible heat associated to the adsorbent and metallic parts, respectively. For a proper understanding of Eq. (10), it should also be recalled here that the adsorbed-phases enthalpies reference is a unitary mass of adsorbent while the gas-phase enthalpies reference is a unitary mass of nitrogen.

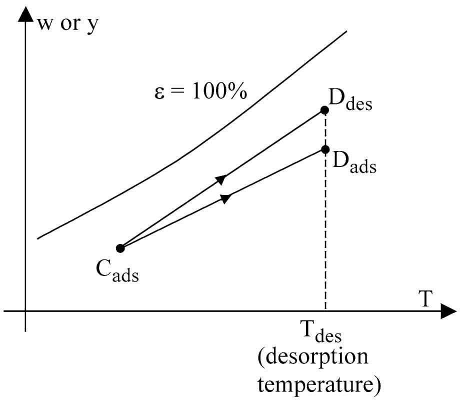

Fig. 6. Graphical representation of a regeneration step.

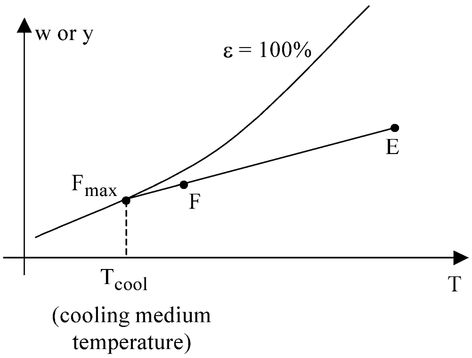

Fig. 7. Graphical representation of a condensation process.

Condensation. The process of VOC condensation (Fig. 7) consists in having a flow (point E) circulating through a cooling coil whose average surface temperature is close to that of the cooling medium and lower than the mixture dew-point temperature, so that a fraction of the VOC vapor actually condenses on the coil. It can be assumed that the mixture is cooled down and tends to a state that can be represented on the diagram as a VOC-saturated mixture ($\varepsilon = 100\%$) at the coil average surface temperature (point $F_{\max}$). Indeed, if the coil transfer area was infinitely long, the outlet temperature of the mixture would reach the coil temperature and the vapor and liquid phases would be in equilibrium. For the same reason as in moist-air psychrometry, the actual outlet state (point F) is represented as a point between the inlet (E) and the ideal outlet ($F_{\max}$). A coil efficiency can thus be defined as:

$$E = \frac{w_E - w_F}{w_E - w_{F_{\max}}} = \frac{h_E - h_F}{h_E - h_{F_{\max}}} \tag{11}$$

According to Le Cloirec [1], the efficiency of such cooling coils for VOC condensation are quite high and can reach up to 98% to 99%.

The energy requirement for this cooling is calculated from the amount of nitrogen flowing through the coil and from the specific enthalpy change:

$$Q_{\text{cool}} = m_{E,\text{N}_2} \cdot (h_E - h_F) \tag{12}$$

4. Practical application of the psychrometric charts: A case study

We consider a nitrogen stream of 3 kg·h^{-1} at 20 °C containing a toluene mole fraction equal to 1000 ppm. This stream must be purified (maximum toluene concentration in the product fixed to 100 ppm) by means of an indirectly heated and cooled TSA process described by Bonjour et al. [6]. This apparatus includes a column of Ambersorb adsorbent (2 kg) which is heated or cooled thanks to an internal heat exchanger (mass of metal = 9 kg). The heat source is steam at 140 °C and the cooling medium is water at 12 °C. A combined process is chosen: it consists in first adsorbing the toluene, then regenerating the adsorber so as to obtained a highly enriched desorbed phase. The enrichment ratio is fixed to 160 (i.e., a mole fraction of 16%), which is easily obtained in the indirectly-heated adsorber technology. The desorbed-phase is lastly condensed on a water-cooled ($T = 12$ °C) coil in order to recover some liquid toluene.

4.1. Determination of the points coordinates on the charts

This combined process is represented under a graphic form in the psychrometric charts on both the molar and the mass-based charts given in Fig. 8. For the sake of clearness and accuracy, the exact coordinates of the points are also given in Table 2. The next paragraphs explain how to obtain the graphs and the coordinates.

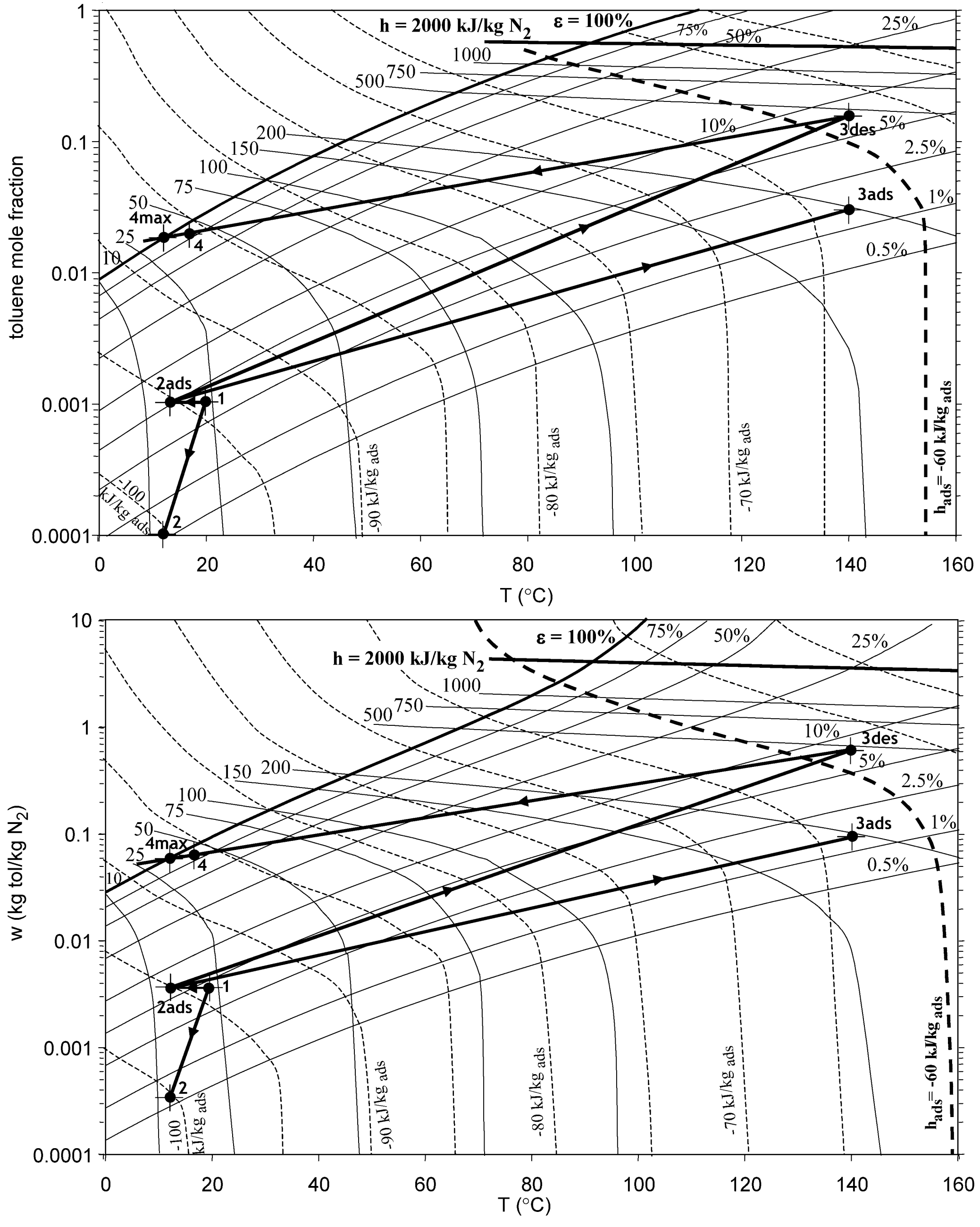

Fig. 8. VOC recovery integrated process presented in the psychrometric charts for nitrogen-toluene mixtures ($P = 101325$ Pa).

Table 2
Coordinates of the points characterizing an integrated process for VOC recovery

Point	T [°C]	w [$g_{tol}\cdot kg_{N_2}^{-1}$]	y [$mol\cdot mol^{-1}$]	ε [%]	h [$kJ\cdot kg_{N_2}^{-1}$ or $^*kJ\cdot kg_{ads}^{-1}$]	q [$kg_{tol}\cdot kg_{ads}^{-1}$]	toluene amount g_{tol}	nitrogen amount kg_{N_2}
1	20	3.29	0.001 (1000 ppm)	4	24	–	262.2	79.69
2_{ads}	12	–	0.001 (interstitial)	–	−95*	0.364	728	negl.
2	12	0.329	0.0001 (100 ppm)	0.75	12	–	26.2	79.69
3_{des}	140	630	0.16	7.5	480	–	236	0.375
3_{ads}	140	–	0.03 (interstitial)	–	−63.4*	0.246	492	negl.
4_{max}	12	61.5	0.0184	100	35.7	–	–	–
4	16.1	72.9	0.0217	93.6	44.6	–	209 (liq) + 27 (vap)	0.375

Points 1 and 2 can be easily located on the molar graph since both the temperature and mole fractions are known. The adsorbed-phase (point 2_{ads}) is in equilibrium with the interstitial gas (1000 ppm) at the temperature at the end of adsorption (i.e. cooling medium, 12 °C). Using the adsorption isotherm, the adsorbed-phase concentration is calculated ($0.364\ kg_{tol}\cdot kg_{ads}^{-1}$, Eqs. (7)–(8)). This also fixes the column capacity, namely 728 g of toluene since the amount of adsorbent is 2 kg. Lastly, the adsorbed-phase enthalpy is read on the graph: $h_{2_{ads}} = -95\ kJ\cdot kg_{ads}^{-1}$.

Point 3_{des} (desorbed phase after regeneration) is identified from the temperature (140 °C) and the mole-fraction (chosen equal to 0.16). The amount of processed toluene must be chosen before continuing the analysis. This choice should be guided by the sought of a trade-off between the energy requirement and the process productivity. If choosing to increase the processed amount, longer regeneration times are necessary, with increased purge gas. This leads to an excess in the heat consumption. On the contrary, a low amount of processed toluene directly means a low productivity. This short reasoning highlights that for a proper design of such combined cycles, a full sensitivity study to that parameter must be performed. For comparable conditions and because of the adsorber performance sensitivity to the choice of operating flow rates during desorption, Clausse [12] retained an amount of 236 g, which is hence the value adopted here. Using the value of the specific mass content of point 3_{des} ($w_{3_{des}} = 0.63\ kg_{tol}\cdot kg_{N_2}^{-1}$), the amount of nitrogen in the desorbed phase is calculated ($m_{3_{des},N_2} = m_{3_{des}}/w_{3_{des}} = 0.375\ kg_{N_2}$). This amount is assimilated to the purge gas if considering that the interstitial nitrogen is negligible.

Point 3_{ads} corresponds to a toluene mass in the column equal to $728 - 236 = 492$ g, i.e. $0.246\ kg_{tol}\cdot kg_{ads}^{-1}$ at $T = 140$ °C. Using the adsorption isotherm, the mole fraction is thus 0.03, which allows to locate point 3_{ads} on the chart, and lastly to read the adsorbed-phase enthalpy ($-63.4\ kJ\cdot kg_{ads}^{-1}$).

As regards the condensation coil, the transfer area average temperature is supposed to be close to that of the cooling water, i.e. 12 °C. It is hence noticeably lower than the dew point temperature of the desorbed-phase, which is found to be 57 °C on the psychrometric chart. Assuming an efficiency of 98% as discussed above, all the points are located on the charts and their coordinates are found. An interesting parameter is the amount of condensed toluene $\Delta w = w_{3_{des}} - w_4 = 0.557\ kg_{tol}\cdot kg_{N_2}^{-1}$, which taking into account the amount of nitrogen in the desorbed phase, yields $m_{3_{des},N_2}\cdot\Delta w = 209$ g of recovered liquid toluene. The amount of toluene remaining under a vapour form is $236 - 209\ g = 27$ g.

Lastly, once the amount of processed toluene is chosen (236 g) and since the inlet and outlet concentrations are fixed (1000 ppm, i.e. $3.29\ g_{tol}\cdot kg_{N_2}^{-1}$, for the feed point 1 and 100 ppm, i.e. $0.329\ g_{tol}\cdot kg_{N_2}^{-1}$ for the effluent point 2), the total amount of toluene entering the adsorber ($m_{1,tol}$) is the amount of processed toluene plus the amount of toluene remaining in the purified effluent ($m_{1,tol} = 236 + 26.2 = 262.2$ g). The corresponding amount of nitrogen, which is supposed to be identical for points 1 and 2 if neglecting the interstitial gas, is hence $m_{1,N_2} = m_{1,tol}/w_1 = m_{2,tol}/w_2 = 79.69$ kg. Because of the chosen mass flow rate, the time of operation for the adsorption step can be evaluated to about 26.6 h.

Compared to adsorber conventional design (including thermal and kinetic effects so that a full numerical simulation is required), the present charts will provide all the more accurate results since the studied system is close to an isothermal single transition system, i.e. the adsorption of a trace compound in an inert carrier gas with no kinetic nor thermal effect as described by Ruthven [13] or Yang [14].

4.2. Energy consumption analysis

A direct application of Eq. (10) allows to calculate the energy requirement for the regeneration step, namely 850 kJ. It is convenient to evaluate the specific heat consumption, i.e. the ratio of the heat to the amount of processed VOC ($m_{3_{des}}$). In the present case, this ratio is $3.6\ MJ\cdot kg^{-1}$ of processed toluene, which lies in the lower part of the range of specific heat consumption of various TSA processes for VOC removal reviewed by LeVan and Schweiger [15]. In addition, this is almost identical to the value computed by Clausse [12] thanks to a rigorous numerical model of the whole adsorber [2] including adsorption kinetics, computation of the velocity and pressure fields etc.: with this model, initially validated from experimental results obtained in various operating conditions [2,6], this ratio was computed to 3.7 $\mathrm{MJ \cdot kg^{-1}}$. This last remark is a clue to assess the validity of the present simplified but practical tool for the energy calculations in adsorbers.

In the indirectly-heated and cooled TSA process, a cooling is necessary after the regeneration step and during the adsorption. The cooling requirement can be obtained by an energy balance analogous to that performed for the regeneration step, from the coordinates of points 3_{ads} (column after the regeneration step), 1 (feed), 2 (product) and 2_{ads} (column after the adsorption step). Including the cooling energy for the adsorbent and metallic parts of the adsorber, the cooling capacity reaches 1325 kJ. Lastly, the cooling requirement for the condensation is calculated from Eq. (12) and is 160 kJ.

This energy consumption analysis shows that the cooling requirement is much higher (1485 kJ) than the heat requirement (850 kJ). This means that even if a combined process using a single heat-pump is operated, half of the heat rejected at the condenser will be wasted. This is nevertheless more recommendable than a completely non-integrated architecture for which the heat is completely wasted. However, another choice of cycle parameters (temperatures, flow rate, enrichment ratio, ...) could probably be made for a higher overall efficiency.

5. Conclusion

Psychrometric-like charts for toluene-nitrogen mixtures in the presence of an adsorbent have been developed. Their use for the representation of unitary operations of VOC recovery processes have been suggested. In spite of highly simplifying assumptions (ideal gases behaviour, ...) with respect to the charts developed by Shallcross or Shallcross and Low [7–9], but taking into account the adsorption equilibrium in the drawing, a reasonable accuracy is obtained when compared to a full numerical simulation of the adsorbers [12]. These charts can be viewed as a new convenient tool for the energy analysis of integrated VOC treatment processes including condensation and temperature-driven adsorbers. This methodology was applied to a case study based on an indirectly heated and cooled adsorber and a heat pump. A proper design of this integrated process allows to use half of the heat available at the heat pump condenser, which is usually wasted.

This new tool should be used in the future for an efficient evaluation of the various combined TSA and heat pump processes evoked in the introductive section, and particularly their energy consumption. The main parameters of influence should be the evaporation and condensation temperatures of the heat pump and the flow rates: these parameters have a major impact on the COefficient of Performance, but also in terms of product purity, process productivity etc. Since a higher temperature difference between desorption and adsorption usually means a higher productivity, but a lower COP, an optimal choice of parameters probably exists for any specific objective.

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