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TECHNICAL NOTE

On Molecular Sieve–Water Interactions

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INTRODUCTION

Adsorption of water vapor on a molecular sieve is probably one of the most common examples of industrial thermal swing adsorption processes. It is therefore not surprising that this has attracted significant attention in the past, and the subject has been studied extensively both experimentally and theoretically. Some of the major contributions include the early work of Carter (1), Nutter and Burnet (2), and Carter and Barrett (3) among others. These systems were recently reviewed by Basmadjian (4) and Ruthven (5). Despite these attempts, there are a number of features which make the interactions between a molecular sieve and water unique in that such interactions are not generally seen on any other adsorbents.

One interesting example of water–molecular sieve interactions relates to the generation of heat which accompanies adsorption. For moisture adsorption on a 13X-type molecular sieve in the vapor phase, the rate of heat generation due to adsorption is approximately equal to the latent heat of water. This is perhaps the reason why vapor-phase moisture adsorption is often described as equivalent to condensation of water within the pores of the adsorbent. It would follow from this argument that there should be no or little heat released when water contacts a molecular sieve in the liquid phase. However, in reality the heat generation due to liquid water contact ranges from large to enormous with a violent reaction depending on the physical nature and other characteristics of the adsorbent.

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The aim of this short note is to describe some of the interesting and hitherto perhaps not fully understood aspects of the regeneration behavior of a bed of molecular sieve initially laden with water vapor.

MOISTURE REGENERATION

It is now well established that the "complete" removal of adsorbed moisture from a molecular sieve would require extremely severe regeneration conditions. Typically, it would require vacuum regeneration at high temperatures of 250°C and greater to evacuate and fully desorb the sieve. Such conditions, although frequently used in laboratories, are extremely difficult to achieve on an industrial scale. Most industrial driers will use less severe conditions for regeneration, implying that a "complete" removal of moisture will never be achieved. Obviously, in the design of industrial drier systems, complete removal of moisture at the end of the regeneration step is neither achieved nor even desired.

It then follows that the optimization of an industrial system would involve only "partial" removal of adsorbed moisture which could be removed relatively easily. The regeneration process therefore leaves behind a permanent deposit of moisture—"residual water"—on the bed. Since regeneration is typically countercurrent to adsorption, the residual water is mainly located at the adsorption inlet end of the bed.

The adsorption profile of water on a "dry" bed is shown in Fig. 1(A). If the sieve is completely regenerated in subsequent cycles, then this profile should result every time at the end of every adsorption step as there is no residual water. However, in practice, the residual water profile elongates during the initial adsorption cycles, as shown in Fig. 1(B). This means that the net amount of water adsorbed during adsorption is greater than

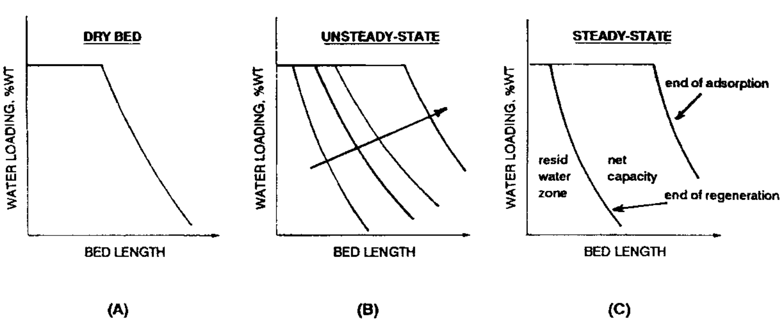

FIG. 1 Water-adsorption profiles.

the net amount of water desorbed during regeneration, so the moist feed carries the moisture a bit further along the bed during these initial adsorption cycles. This is known as the transient unsteady-state regeneration. However, after a few cycles, a point is reached where the degree of regeneration is sufficient to prevent further migration of moisture, and a steady state is reached. At this time the net amounts of water adsorbed and desorbed are exactly the same and the adsorption profiles remain unchanged from cycle to cycle. The regeneration can be termed "adequate," and steady-state profiles for both adsorption and regeneration are achieved as shown in Fig. 1(C). It is important to note that a slight change in the regeneration conditions is enough to disturb the steady state. A new steady state would then be established, albeit with a different moisture profile in the bed.

Most industrial thermal swing designs would attempt to operate at "adequate" regeneration conditions. In order to confidently calculate the "adequate" regeneration conditions, it is important to understand the residual water behavior for a given set of regeneration conditions. Some of the main factors which affect the residual water are described below.

Degree of Regeneration

There are three parameters which influence the degree of regeneration. These are the regeneration temperature, the regeneration flow, and the regeneration time. It is now well established that there is an optimum combination of the three parameters which controls the extent of regeneration and the residual water profile. The regeneration temperature or the maximum temperature achieved at the bed outlet during regeneration step are not the only parameters.

Total Regeneration Heat Input

In most designs of driers the regeneration energy requirement is calculated using the net amount of water to be desorbed and the heat of desorption for water. To this is added the heat requirement to heat the vessel and adsorbent to the desired temperature. However, it is not enough to deliver the total heat as the extent of regeneration depends on a combination of regeneration flow, temperature, and time. For example, consider the values given in Table 1.

It is interesting to note that although the amount of heat delivered in all cases given in Table 1 is exactly the same, the actual residual water may be different in each case. For example, more effective regeneration may be possible at a regeneration flow of 4000 sm^3/h, a regeneration temperature of 150°C, and a heating time of 1.335 hours than at a regeneration

TABLE 1

Flow (sm^3/h)[a]	Temperature (°C)	Heating time (h)
2000	200	2.00
	150	2.67
4000	200	1.00
	150	1.335

[a] Defined at 1.013 bar a and 15.5°C.

flow of 2000 sm^3/h, a regeneration temperature of 200°C, and a heating time of 2 hours. In terms of designs, this behavior would mean that regeneration strategies involving high flow/low temperature and low flow/high temperature for identical feed conditions may actually have different bed designs.

Multicomponent Systems

If the system has to adsorb any other nonpolar component in addition to water, then the analysis becomes more interesting. Since water vapor would tend to displace the weakly adsorbed component, the concentration of the weakly adsorbed component would actually increase in the bed. Designs involving multicomponent systems with water as one of the components would have to recognize this fact so that necessary adjustments can be made in the design. The peak concentration of the weakly adsorbed component in the bed is the key information required to incorporate the effect of displacement due to water.

During the period when the steady-state conditions have not been fully developed, i.e., the net water adsorbed is greater than the net water desorbed, the peak concentration of the weakly adsorbed component will be greater. This is because the residual water front advances during this period, causing appreciable displacement. However, as the steady state is approached, the peak concentration starts to reduce. This is because the sieve now has some residual moisture on it which reduces the adsorption of the weakly adsorbed component. The sieve has a very small amount of the weakly adsorbed component on it to be displaced.

Another interesting feature is that the single component adsorption of a weakly adsorbed component is actually less on a wet bed than on a dry bed with multicomponent adsorption. This is because there is no displacement effect on a wet bed, and therefore the favorable effect of high concentration on the equilibrium isotherm cannot be considered. Obviously, multicomponent adsorption on a wet bed is very difficult to analyze, although it represents reality.

CONCLUSION

Interaction of water and a molecular sieve is unique and interesting in many aspects. The existence and dominance of residual moisture makes it different from other similar drying systems employing other adsorbents such as activated alumina or silica gel. Some of these aspects are described in this note. The mechanism of water adsorption and its subsequent regeneration from a bed of molecular sieve is not only of fundamental interest but also has significance for industry. In any design of industrial driers employing a molecular sieve or any other adsorption unit involving multicomponent adsorption in the presence of water vapor, these aspects have to be considered to come up with a reliable and robust design. Failure to appreciate these aspects could result in the under or over design of such units.

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