ABSTRACT

The dynamics of the adsorption of carbon dioxide and moisture on molecular sieves 5A and 13X have been investigated. The adsorption breakthrough data are generated through experimental investigation and are analysed using a simplified theoretical model for multi-component adsorption. The model utilised Langmuir type multi-component adsorption isotherm relationship. The isotherm parameters are obtained from the literature.

The effect of non-dimensional parameters like adsorbate inlet concentration, particle Reynolds number, Schmidt number, Prandtl number, Kutateladze number, Sherwood number, bed diameter to bed length ratio etc. are studied in detail for the single component adsorption. The shape and appearance of the breakthroughs are analysed with respect to the above mentioned parameters.

In case of multi-component adsorption, the roll up behaviour of carbon dioxide in presence of moisture is obtained through experiment. The parameters which give multi-component effect are varied theoretically and their effects on the roll up behaviour are analysed.

Finally, from the energy conservation view point, the irreversibility analysis of the adsorption system is performed. A theoretical model and a methodology has been developed to calculate the rate of entropy generation due to mass transport, momentum transport and thermal effects. The entropy generation due to heat transfer has been found to be of largest magnitude and attributes mainly to the total entropy generation. The effects of various important parameters like adsorbate inlet concentration, particle Reynolds number, Schmidt number, Kutateladze number, Sherwood number, bed diameter to bed length ratio etc. on the total entropy generation of the process are analysed.

KEY WORDS

Adsorption, Adsorbate, Adsorbent, Breakpoint, Breakthrough, Entropy, Isotherm, Irreversibility, Kutateladze Number, Roll Up

SUMMARY

The dissertation has been presented mainly in five chapters and their contents are briefly presented below.

CHAPTER - I

This section deals with the extensive survey of literature on single and multi-component adsorption in various adsorbents. Various models have been developed on the basis of molecular diffusion, different forms of adsorption isotherms, hydrodynamics of the system, heat transfer due to heat of adsorption etc. The experimentally determined breakthrough curves have been explained by the developed models with various degrees of accuracy. Limitations of different models have been discussed to account for the discrepancy in correlating the experimental data.

CHAPTER - II

Chapter - II presents the development of a theoretical model for multi-component adiabatic adsorption with porous molecular sieves packed in a vertical column. Based on suitable assumptions to reduce the complexity of the system, the model has been presented in the form of mass and energy balances for the adsorbate fluid and solid adsorbent, coupled with adsorption isotherm of components.

The mass transfer aspect of the adsorption process in terms of molecular diffusion, pore diffusion has been taken into consideration and these are coupled in the form of resistances to predict the overall mass transfer coefficient. Gas to particle heat transfer coefficient has been assumed to be a constant for a narrow temperature range of study and has been adopted from the literature.

The model equations have been solved by making them first dimensionless and the coupled partial differential equations are converted into simple ordinary differential equations after breaking the spatial derivatives by central difference techniques and are solved explicitly using backward difference approach. The stability of the solution is monitored continuously using stiffness ratio.

CHAPTER - III

Experimental scheme and procedure have been presented in this chapter. The set-up consists of a vertical adsorption column of 50 mm dia and 700 mm length. The adsorbents used were type 5A (Linde molecular sieve) and type 13X (ACC molecular sieves). The height of the packing with adsorbents in the adsorber column has been varied. The concentration of the adsorbate, moisture in the N_2 stream, has been adjusted by saturating the N_2 stream in a series of water bubblers immersed in a constant temperature bath. Carbon dioxide from a cylinder was metered and mixed with metered N_2 flow with or without water saturation and then introduced into the bottom of the adsorber column. The inlet and outlet concentrations of moisture were monitored by absorbing moisture through a series of tubes filled with magnesium perchlorate for a definite length of time. The carbon dioxide concentration in the feed as well as in the effluent were measured on line with the help of a carbon dioxide analyser.

The variables studied were inlet concentrations of the adsorbates, residence times, types of adsorbents, height of packing, the ratio of two adsorbates.

CHAPTER - IV

This chapter deals with experimental results presented in figures and tables. The breakthrough curves have been plotted with dimensionless outlet concentration against dimensionless times. The theoretical models have been simulated with the experimental data, using estimated and adopted parameter values(from literature) for the systems. The adequacy of the fit of the data with the theoretical model has been tested. Various dimensionless parameters like inlet concentration of the adsorbate, particle Reynolds number, Schmidt number, Sherwood number, Kutateladze number, bed diameter to bed length ratio etc. have been studied to find their effects on the breakthrough curves.

CHAPTER - V

This chapter contains thermodynamic study of the adsorption system. A theoretical model has been developed for adsorption process for the total entropy generation of the process and an attempt has been made to obtain the effects of pertinent process variables on the entropy generation of the process. Total entropy generation for adsorption of gases has been shown to be the sum total from three sources like mass transfer, fluid flow and thermal effect. It has been found that the total entropy generation due to thermal effect is much higher than that due to mass transfer or fluid flow. The total entropy generations due to mass transfer and fluid flow are found to be of same order of magnitude. Various dimensionless parameters like inlet concentration of the adsorbate, particle Reynolds number, Schmidt number, Sherwood number, Kutateladze number, bed diameter to bed length ratio have been studied to find their effects on the entropy generation of the process.

The major inferences can be drawn from the present study are

1. Linde molecular sieve has much higher adsorption capacity for both carbon dioxide as well as moisture, compared to the ACC 13X molecular sieve.
2. Compared to carbon dioxide, moisture has been found to be preferentially adsorbed component. Roll-up behaviour in the concentration breakthrough curves of carbon dioxide has been distinctly observed in case of simultaneous adsorption of carbon dioxide and moisture.
3. Moisture adsorption behaviour is not affected significantly in presence of carbon dioxide during their simultaneous adsorption. But presence of moisture plays an important role on the adsorption characteristics of carbon dioxide.
4. For simultaneous adsorption of carbon dioxide and moisture, higher Rep reduces the roll-up of carbon dioxide.
5. The theoretical model based on the Linear Driving Force approximation, has predicted the adsorption system behaviour for single component as well as multi-component adsorption studies with a fair degree of accuracy.
6. Above a certain value of inlet adsorbate concentration, an increase in Ku decreases the fluid and solid phase temperature in the bed. In case of multi-component adsorption, increase of moisture Ku number significantly decreases the adsorption behaviour of both the components.
7. For $Ts_o/Tg_o < 1.0$, both adsorption and desorption processes take place simultaneously within the bed leading to a temperature plateau as well as roll-up of the adsorbate.
8. Entropy generation due to heat transfer in adiabatic adsorption process is much higher than those of the other effects.
9. Except momentum transport, entropy generation due to other effects reaches a steady state value towards the end of the adsorption process, whereas, entropy generation due to momentum transport goes on increasing.