

Separation of Mixtures at Nano Length Scales: Blow Torch and Levitation Effect[†]A. V. Anil Kumar,[‡] S. Yashonath,^{*,‡,§,⊥} and G. Ananthakrishna^{§,||,⊥}

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A new conceptual basis for the separation of multicomponent molecular mixtures is proposed. A separation method where different components of the mixtures are driven in opposite directions is realized by a judicious combination of two effects, viz., levitation and blow torch effects. Monte Carlo simulations of two Lennard–Jones binary mixtures with different-sized components are shown to be separated well if at least one of the components lies in the anomalous regime and the others lie in the linear regime. A separation factor of 10^8 is obtained on nano length scales as compared to 10^3 , obtainable through conventional methods of separation on macrolength scales.

1. Introduction

Many physical properties of fluids confined to porous solids are significantly different from that of bulk systems.^{1–3} These differences arise from: (i) the presence of a large fraction of atoms at the interfaces, (ii) confinement effects, and (iii) heterogeneity of the surfaces. The confining walls can have considerable influence on both the static as well as the dynamic properties of confined fluid. Spatial heterogeneity, common to porous solids such as zeolites, can also have considerable influence on transport properties. Here, the spatial heterogeneity refers to the differences in properties of guests in different spatial regions. For instance, it is well-known that viscosity of a few monolayers of confined fluid is very high and drops to bulk value as the number of monolayers of the confined fluid increases (decreasing typically by a factor of 10 for every layer).⁴ This aspect is of considerable interest in understanding boundary lubrication.⁵ Further, previous studies have shown⁶ that regions close to the internal wall of a zeolitic cage is significantly lower in guest–host potential energy of interaction as compared to the region near the cage center. This result also holds for any other types of void including a cylindrical (straight or sinusoidal) channel.

One interesting consequence of such heterogeneity is the levitation effect (see below), which refers to a maximum in the self-diffusivity of the diffusant when its size is comparable to the pore size.⁷ Levitation effect refers to the anomaly in diffusivity that has been observed in porous solids. Self-diffusivity D exhibits a surprising dependence on the size of the guest species, σ_{gg} , the Lennard–Jones guest–guest interaction parameter. At small σ_{gg} , D is linearly proportional to $1/\sigma_{\text{gg}}^2$. This is the linear regime. At larger σ_{gg} , D shows a pronounced peak (seen Figure 1), which is referred to as the anomalous or the levitating regime.⁷ This behavior is observed in all types of porous solids irrespective of the geometrical and topological details of the pore network.

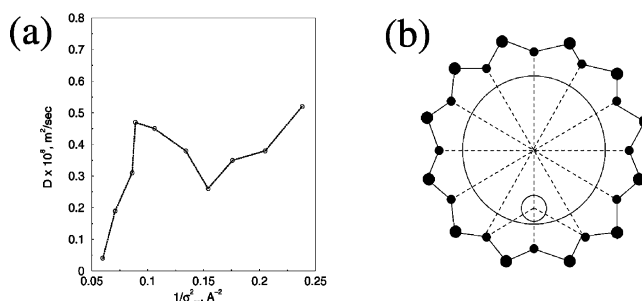


Figure 1. (a) Plot of self-diffusivity vs $1/\sigma_{\text{gg}}^2$. (b) Twelve-membered ring of zeolite NaY is shown along with two guests, one of similar size and another of smaller size. In the case of the former, dispersion interactions from any side of the host are equal and opposite to that due to the diagonally opposite side.⁷ This results in negligible force on the guest. In the case of a smaller particle, this is not the case.

A dimensionless parameter⁷

$$\gamma = \frac{2^{1/6} \cdot \sigma_{\text{gh}}}{\sigma_{\text{w}}/2} \quad (1)$$

called the levitation parameter may be defined. Here, σ_{w} is the window diameter and σ_{gh} is the guest–host Lennard–Jones interaction parameter. The anomalous regime is seen when γ is close to unity and the linear regime for values of $\gamma \ll 1$. The maximum in self-diffusivity has its origin in the fortuitous cancellation of the dispersion forces on the guest or diffusant due to the host. Such an unexpected cancellation of forces arising from the host porous medium occurs when the size of the guest is comparable to the void size (see Figure 1b). Frictional forces on the guest are then lowest, and this results in an increase in D . Under these conditions, it is seen that the potential energy landscape is rather flat, with only smaller undulations.⁸ The magnitude of the peak in D is dependent on the temperature and degree of disorder in the void network.^{8,9} Generally, in most guest–host systems, γ is small and hence they lie in the linear regime. To realize the anomalous regime, a careful choice of the host system for a given guest or mixture is, therefore, necessary.

Another consequence of chemical as well as spatial heterogeneity is significant variations in temperature from one region

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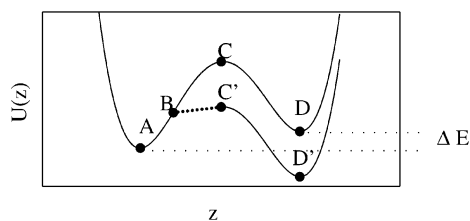


Figure 2. The effect of the hot zone between B and C in the potential ABCD is to effectively lower D to D'. The resulting "effective potential" is now given by ABC'D'.

to another region within zeolites. For example, zeolites are well-known heterogeneous catalysts and these cause local release or absorption of heat near catalytic reaction centers. Even adsorption near chemisorption or physisorption sites can lead to variations in temperature within zeolites.¹⁰ The duration over which such variations in temperature persist or the relative magnitude of change in temperature may be small or large depending on the thermal conductivity of zeolites. The thermal conductivity of zeolite itself might depend on a number of factors, such as the Si/Al ratio, nature of extraframework cations, amount of water, etc. However, what is self-evident is that such variations in temperature can exist within zeolites.

The effect of inhomogeneous temperature has been previously studied by Landauer in a seminal paper¹¹ which now goes by the name "blow torch" effect. Briefly, he showed that introduction of a hot spot between a lower-lying minimum and barrier maximum of a bistable potential can raise the population of the higher-lying minimum relative to the lower-lying minimum over and above that given by the Boltzmann factor.

Because the blow torch effect is rather counter intuitive, following Landauer,¹¹ we illustrate the effect of a nonuniform temperature bath on the relative populations of competing local energy minima for a bistable or double well potential $U(z)$. Consider the motion of an overdamped particle in the potential $U(z)$, shown by the curve ABCD in Figure 2, subject to a uniform temperature T_0 along the coordinate. Then, the probability of finding a particle at z is $P(z) \sim \exp(-U(z)/k_B T_0)$. Clearly, the probability at A is higher than that at D. Now consider raising the temperature of the region BC to T_b . Then $P(z) \sim \exp(-U(z)/k_B T_b)$ in BC is clearly much smaller than the probability $P(z)$ at lower temperature $T = T_0$, given that $U(z) < 0$. Now let us consider a situation when only $P(z)$ is given and one wishes to find the "effective potential" that determines this $P(z)$. Clearly, one can invert the original expression for $P(z)$ and regard the "potential" to be given by $U(z)/k_B T = -\ln P(z)$. Thus, on raising the temperature to T_b , the decrease in $P(z)$ in BC implies $\ln(P(z))$ is flatter in BC. This is equivalent to modifying the "potential" to a flatter curve BC'. Regions outside of BC will be altered only indirectly through the change in the normalization constant obtained by integrating over the whole region. Because the probability $P(z)$ is essentially unaffected in other regions, the "effective potential" denoted by the curve outside the region BC will be almost unaltered except that the curve CD would start at C' and end at D', such that $U(z_C) - U(z_D) = U(z_{C'}) - U(z_{D'})$. Thus, the minimum at D is brought down relative to A. Consequently, the probability at z_D , $P(z_D)$ is higher than that at the lower minimum z_A .

Most of the studies on blow torch effect deal with steady-state properties.^{12,13} Only recently, kinetic aspects have been studied¹⁴ for an idealized situation. More recently, we have demonstrated a more practical realization of the blow torch effect in the case of a zeolite.¹⁵

Here, we investigate the effect of combining both of these two effects (the levitation and blow torch effects). The system

of interest is a binary molecular mixture confined to a zeolite. We show that when the two effects are combined judiciously, it can lead to an excellent separation of the two components of the mixture. We have carried out Monte Carlo simulations of (i) Lennard–Jones and (ii) Ar–Ne mixtures confined in zeolite A. The main purpose of this work is to introduce a new conceptual basis that can lead to superior separations as compared to existing methods. The question of practical realization of the conditions under which such excellent separation is obtained are only dealt with briefly. With the rapid advances in experimental nano science and technology, it may not be long before the experimental conditions are actually realized. Our simulations suggest that it is possible to realize separation factors that are quantitatively superior by several orders of magnitude to the existing methods. The length of the separation column over which the mixture traverses is reduced significantly from macro- to microscopic dimensions.

2. Methods

Consider a fluid mixture confined to NaCaA zeolite (composition $\text{Na}_{32}\text{Ca}_{32}\text{Si}_{96}\text{Al}_{96}\text{O}_{384}$, Si/Al = 1.0). Space group, $Fm\bar{3}c$, of zeolite A, with a lattice parameter $a = 24.55 \text{ \AA}$ reported by Pluth et al., has been employed.^{16,17} Large ($\approx 11.4 \text{ \AA}$ diameter) cages (the supercages) are interconnected to six other supercages along the crystallographic axes via 8-ring windows of significantly narrower diameter ($\approx 4.5 \text{ \AA}$). The distance between two planes of 8-ring windows is given by half of the lattice parameter $d_w = a/2 = 12.275 \text{ \AA}$. We introduce a hot spot just prior to the window along the c -direction. The precise location of the hot spot, etc., are indicated below. Such a hot spot can arise, for example, because of the presence of a heterogeneous reaction site or a chemisorption site or even a physisorption site, as we have recently shown.¹⁵ The presence of a hot zone aids the molecules to surmount a barrier more easily. Because the rate-determining step for diffusion is the passage through this bottleneck, the distance from this plane is taken as the "diffusion coordinate", (akin to "reaction coordinate"). The progress of the passage through the bottleneck is indicated by this distance. In the present simulation, the start of the hot spot is at a distance d from the plane of the 8-ring window of zeolite A separating two cages. The hot spot has a width w (see Figure 3). The hot spot is placed to the left of the window plane of only those windows that lie in the xy plane, and those windows whose planes lie in xz or yz planes are "ordinary" windows without any hot spot to their left. The "diffusion coordinate" in this setup is, therefore, simply the z direction.

Previous studies have shown⁷ that the average potential energy (PE) landscape for particles in linear ($\gamma \ll 1$), and anomalous ($\gamma \approx 1$) regimes are substantially different. For the linear regime, the potential energy maximum and minimum are located respectively at the bottleneck (8-ring window) and the cage. For the anomalous regime, they are located at the cage and the bottleneck, respectively (see Figure 3).⁷

We describe the zeolite and mixture of gases interacting via the Lennard–Jones potential $\phi(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$. The total interaction energy of the system consists of the guest–guest, $\phi_{gg}(r)$, and guest–zeolite, $\phi_{gh}(r)$, terms:

$$\Phi = \sum_{i=1}^N \sum_{j=1}^N \phi_{gg} + \sum_{i=1}^N \sum_{j=1}^{N_z} \phi_{gh}$$

where N and N_z are the number of guest and zeolite atoms, respectively. In the absence of appropriate techniques for including nonuniformity in temperature (that is, in maintaining

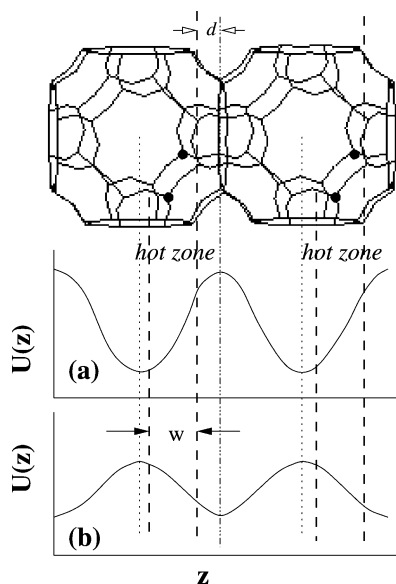


Figure 3. Two cages of zeolite NaCaA with the location of the chemisorption or physisorption or reactive sites (filled circles). The potential energy variation along the z direction for particles in the (a) linear and (b) anomalous regime are shown. The location of the hot zone is indicated by the boundaries, shown by the dashed vertical lines. In the Monte Carlo simulations, the start of the hot zone H is located 1.2775 \AA from the window plane (indicated by d) and has a width of 2 \AA (indicated by w in the figure), extending up to 3.2775 \AA from the window plane. Note that the hot zones repeat with the same periodicity as the α -cages along the z direction and are located at the same place relative to the windows.

steady-state excess temperature in a localized region) within the existing molecular dynamics algorithms, we employ a modified Metropolis Monte Carlo algorithm in the canonical ensemble.⁴ In other words, there is no way of introducing temperature inhomogeneities within the existing molecular dynamics simulation method. On the other hand, the implementation of the importance sampling within Monte Carlo is straightforward. The zeolite atoms are treated as rigid, and no attempts are made to displace them. A new position for the guest particle is obtained randomly through displacement moves in the usual fashion. The probabilities for the acceptance, however, depend on the region in which the guest lies before and after the displacement. The probability associated with the position of the guest are different for the normal and hot zones:

$$P(\mathbf{r}_i) \propto \exp(-U(\mathbf{r}_i)/kT_b) \text{ if } \mathbf{r}_i \in H$$

$$P(\mathbf{r}_i) \propto \exp(-U(\mathbf{r}_i)/kT_0) \text{ if } \mathbf{r}_i \notin H$$

where the hot zone is indicated by H . If the i th particle is in the hot zone, then the probability is calculated with temperature T_b . If the i th particle is outside of the hot zone, then the probability is calculated with temperature T_0 . If a particle is located in the region where temperature is T_0 prior to the displacement move, and is located in the hot zone H after the displacement, then the transition probability for this move will be given by

$$W(r_i \rightarrow (r'_i \in H)) = \exp(-[U(r'_i)/T_0 - U(r_i)/T_b]/kT_0T_b)$$

If, on the other hand, the particle is in the hot zone H prior to displacement and is out of the hot zone after the displacement, then

$$W((r_i \in H) \rightarrow r'_i) = \exp(-[U(r_i)/T_b - U(r'_i)/T_0]/kT_0T_b)$$

Calculations have been carried out at a temperature of $T_0 = 140 \text{ K}$ with temperature of the hot spot $T_b = 420 \text{ K}$. We carry out two sets of simulations, the first (set A) relating to idealized particles to illustrate the basic effect, and the second (set B) on a realistic mixture of neon–argon. Both are modeled in terms of their Lennard–Jones potential parameters. A 1:1 mixture with a total of 256 particles corresponding to a concentration of $c = 1/\text{cage}$ (of either type chosen randomly), diffusing within zeolite NaCaA, has been simulated. The system consists of $2 \times 2 \times 8$ unit cells of zeolite A, each unit cell containing 8 cages ($l_z = 8 \times a = 196.4 \text{ \AA}$). Periodic boundary conditions are imposed along the x and y directions. Along the z direction, repulsive ($1/r^{12}$) walls are placed at $z = 0$ and $z = l_z$. For the set A itself, we carry out two simulations LR and AR, defined by their respective parameters: the mixture LR, consisting of particles with $\sigma_{\text{gg}} = 2.05$ and 2.38 \AA , and mixture AR with $\sigma_{\text{gg}} = 2.38$ and 3.34 \AA . For mixture LR, both of the components lie in the linear regime.⁷ For mixtures AR, one of the two components, viz., $\sigma_{\text{gg}} = 3.34 \text{ \AA}$, lies in the anomalous or levitating regime.⁷ The Lennard–Jones interaction parameter $\epsilon_{\text{gg}} = 0.997729 \text{ kJ/mol}$ for all the guests. For set B, simulations of neon–argon mixture, the parameters are:¹⁸ $\sigma_{\text{Ne-Ne}} = 2.72 \text{ \AA}$, $\epsilon_{\text{Ne-Ne}} = 0.3908 \text{ kJ/mol}$, $\sigma_{\text{Ar-Ar}} = 3.41 \text{ \AA}$, and $\epsilon_{\text{Ar-Ar}} = 0.9977 \text{ kJ/mol}$. Interactions between the guest molecule and the zeolite was considered as discussed elsewhere¹⁹ by including interactions between zeolite atoms O, Na, Ca, and the guest. Initially, a single particle of either type is placed in each cage, corresponding to the equilibrium distribution in the absence of blow torch. There are two cages along each of the x , y , and z directions per unit cell. A hot spot is placed at a distance of $d = 1.2775 \text{ \AA}$ to the left of the 8-ring window along the z direction (see Figure 3). The width of the hot spot $w = 2 \text{ \AA}$. As the simulation cell consists of $2 \times 2 \times 8$ unit cells of zeolite A, the hot zones are located periodically in the interval $(na/2 - 3.2775, na/2 - 1.2775)$, $n = 1, 2, \dots, 16$ to the left of the 16 windows in the xy plane in 8 unit cells along the z direction. Simulations are of 6×10^5 MC steps, which includes an initial period of 5×10^5 MC steps required for reaching a steady state. Average properties are calculated over 1×10^5 MC steps.

3. Results and Discussion

We first discuss the results of LR mixture of set A (with $\sigma_{\text{gg}} = 2.05$ and 2.38 \AA). Figure 4 shows the density profile along the z direction, $n_i(z)$ for $i = 1, 2$, along with the logarithm of the ratio $n_1(z)/n_2(z)$ along the z direction. Clearly, there is hardly any separation of the two components. The separation factor²⁰ is of the order of unity. In contrast, the plots of $n_i(z)$ for $i = 1, 2$ and $\ln(n_1(z)/n_2(z))$ for the mixture AR (with $\sigma_{\text{gg}} = 2.38$ and 3.34 \AA) show a high degree of separation (Figure 5). The component corresponding to $\sigma_{\text{gg}} = 2.38 \text{ \AA}$ is driven to the right and accumulates at one end, while the other component with $\sigma_{\text{gg}} = 3.34 \text{ \AA}$ is driven to the left. At one extreme, the ratio $n_1(z)/n_2(z)$ is 72.61, while at the other extreme, a value of 0.01329 is obtained. This corresponds to a high separation factor²⁰ $\alpha = 5463$.

We now demonstrate the applicability of this method to the separation of a mixture of real gases, namely, Ne–Ar rare gas mixture, by using zeolite NaCaA as the porous host. A plot of $n_{\text{Ar}}(z)$, $n_{\text{Ne}}(z)$ and their ratio $\ln(n_{\text{Ar}}(z)/n_{\text{Ne}}(z))$ as a function z is shown in Figure 6. Clearly, there is an excellent separation of the two components. At the left end, the ratio $n_{\text{Ar}}(z)/n_{\text{Ne}}(z)$ is 301.81, while at the right extreme, it is 0.02255. The resulting separation factor is 1.338×10^6 . Further, use of even a few more unit cells of zeolite can enhance the separation factor by several orders of magnitude.

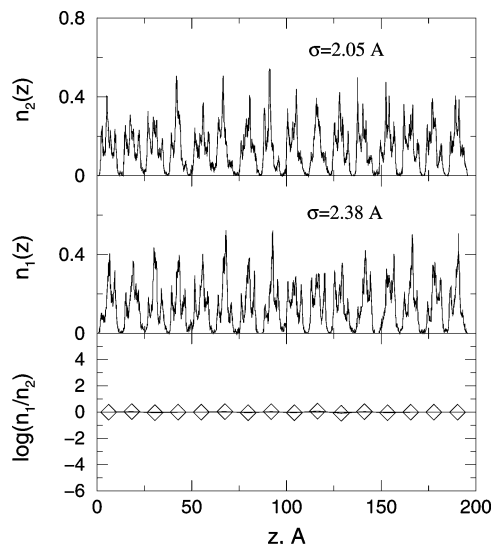


Figure 4. Variation in density along the z direction of two components in mixture LR, where both of the components are from the linear regime. Also shown are the ratio $\ln(n_1(z)/n_2(z))$.

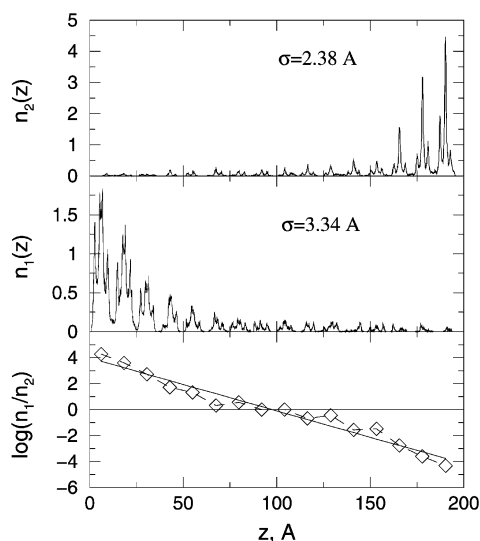


Figure 5. Variation in density along the z direction for the mixture consisting of an anomalous and a linear regime component (AR) and the ratio $\ln(n_1(z)/n_2(z))$. A straight-line fit to $\ln(n_1(z)/n_2(z))$ has been used to obtain parameters in eq 2.

It is clear from Figures 5 and 6 that a straight line fit to the plot of $\ln(n_1(l)/n_2(l)) - l$ (or $\ln(n_{Ar}(l)/n_{Ne}(l)) - l$) provides a good approximation. Therefore, the ratio $n_1(l)/n_2(l)$ (or $n_{Ar}(l)/n_{Ne}(l)$) decreases in an exponential way and can be fitted to:

$$\frac{n_1}{n_2} = e^{-l/l_c + c} \quad (2)$$

where l is the length of the separation column and l_c and c are constants. $l_c = 22.823$ Å (mixture AR) and 20.6698 Å (Ne–Ar), and $c = 4.2851$ (mixture AR) and 5.710 (Ne–Ar mixture), respectively. Here, we have fixed the magnitude of $n_1/n_2(z = 0)$ to e^c . It follows from eq 2 that the separation factor²⁰ for a separation column of length l_z may be written

$$\alpha = \frac{n_1/n_2(z = l_z)}{n_1/n_2(z = 0)} = e^{-l_z/l_c} \quad (3)$$

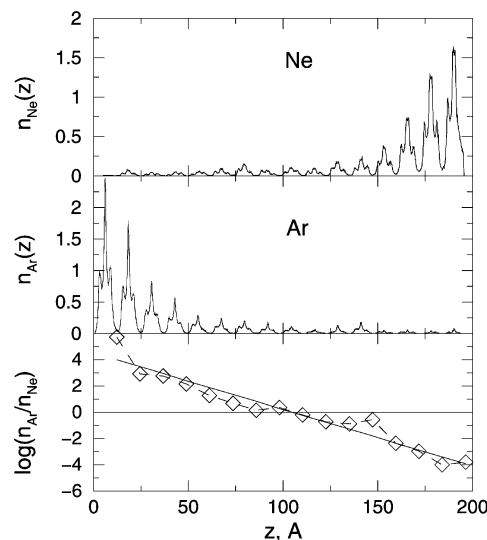


Figure 6. Variation in density along the z direction for Ne–Ar mixture for component Ar, Ne, and the ratio $\ln(n_{Ar}(z)/n_{Ne}(z))$. A straight-line fit to $\ln(n_{Ar}(z)/n_{Ne}(z))$ has been used to obtain parameters in eq 2.

TABLE 1: The Value of γ Defined in Eq 1 for Different Guests in Zeolite A

$\sigma_{gg}, \text{Å}$	γ
2.05	0.73
2.38	0.79
3.34	0.94
2.72 (Ne)	0.84
3.405 (Ar)	0.95

The resulting value for α on doubling the column length to $l_z = 392.8$ Å 1.79×10^8 , which is more than 2 orders of magnitude improvement over the value 1.338×10^6 obtained for Ne/Ar mixture for $l_z = 196.4$ Å. In conventional methods of separation, the separation factor at best varies linearly with the length of the column.²¹ The present method is, therefore, capable of providing better than parts per billion purity with columns of microscopic dimensions. The efficiency of separation is also expected to be several orders of magnitude better than obtained from conventional methods.

These results can be understood by considering the nature of the potential energy landscape for particles in the linear and anomalous regimes (Figure 3) and the position of the hot spots. Table 1 lists the values of γ for the components of the LR, AR, and Ne–Ar mixtures. In the case of LR mixture, both components fall in the linear regime as their γ values are much less than unity. For these particles, the maxima in the potential energy landscape are at the windows ($z_n = nd_w$ where n is an interger) just to the right of the hot spots (see Figure 3a). Thus, the effect of the hot spot is to increase the escape rate over the barrier located to the right of the hot spot. Stationary populations of both species in the presence of hot spots are soon established, which is nearly uniform. In contrast, for the AR mixture or Ne–Ar mixture (Table 1), while one component lies in the linear regime (γ much less than unity), the other component is in the anomalous regime with $\gamma \sim 1$. For the latter, the potential maxima are located at the cages ($z_n = (2n + 1)d_w/2$, n is an integer), which are immediately to the left of the hot spot. Thus, the hot spot has the effect of driving these particles to the left, while the other component (in the linear regime) is driven to the right. Because the hot spots are located at periodic positions, the eventual effect is to accumulate particles of each type at the left and right extremes, respectively. This is what is seen in Figures 5 and 6.

TABLE 2: Choice of Zeolite for Hydrocarbon and Other Mixtures Chosen So That One of the Components Has a Value of γ Close to Unity in Zeolite Faujasite (with $\sigma_w = 10.11$ Å)

guest	$2^{7/6}\sigma_{gh}$	γ
isopentane	10.03	0.995
<i>n</i> -hexane	8.08	0.799
<i>n</i> -butane	8.08	0.799
CCl ₄	8.39	0.829
CF ₄	6.99	0.692

It is clear that, unlike conventional²¹ or the earlier method of separation that depend only on the levitation effect,²² our present method depends crucially on the interplay of two factors, namely, the levitation and blow torch effects. It is applicable to mixtures where the two components differ in size. The realization of the levitation effect requires a careful choice of the porous host, which depends on a few pertinent points. Previous studies show that the enhancement of D within the anomalous regime extends over a reasonably large range of σ_{gg} .⁸ This provides considerable flexibility in the choice of the host system over which the anomalous regime can be realized. There exist in nature a number of known porous solids¹⁰ with a wide variation in pore dimensions. Further, it is also possible to vary the pore dimensions of these solids through, for instance, substitution of framework ions. Substitution of Si by Al or Si by P or Al by Ti can alter the pore dimensions.²³

Table 2 illustrates the choice of the zeolite as the host for a few realistic molecules.¹⁰ For the hydrocarbon mixture consisting of *n*-hexane, *n*-butane, and isopentane, it is seen that isopentane alone has a γ close to unity. Therefore, in the application of the present method to this mixture, isopentane alone would be driven to the left, while the other two would be driven to the right. Thus, it is possible to separate out isopentane from other components. The other binary mixture of CCl₄ and CF₄, the component with γ value closer to unity would be driven to left and the other component with $\gamma \ll 1$ will be driven to the right.

The realization of the hot spot may be more difficult. This can be done if, for example, a specific chemical group can be attached to the oxygen of the zeolite framework at the place where the hot spot is desired. The chemical group can then be vibrationally excited by exposing it to infrared radiation of appropriate wavelength. Thermal deexcitation of the excited group would provide a constant heat source. The system would soon reach a steady state nonequilibrium state with a temperature gradient. The location of the chemical group has to be asymmetric with respect to the barrier, i.e., placed only on one side of the barrier. For this, use of a noncentrosymmetric zeolite may be necessary.

A few points relating to the choice of the different parameters in the present study are worth discussing. We have employed a rather high temperature for the hot zone, viz., $T_h = 420$ K. Such a high temperature for the hot zone is probably difficult to realize in practice. Further, such a large temperature for the hot zone is not required to see the observed separation. Suppose the temperature of the hot zone is decreased from $T_h = 420$ K to something lower, say $T_h = 210$ K. In this case, the driving force that drives the component of the linear regime to the right and the component of the anomalous regime to the left is lowered. As a result, the required separation of, say, 1 in 10^8 , will be achieved not just over 16 unit cells of zeolite A, but instead, it will be achieved over a longer column of zeolite. The total length of zeolite column required will still be, however, on a nano length scale. Here, we have chosen to employ a higher

temperature T_h to minimize the length of the column of zeolite, which will lead to considerable reduction in computational time. In conclusion, we have demonstrated the utility of the levitation and blow torch effects to separation of mixtures in the context of zeolites.²⁴ At a fundamental level, this method of separation is different from conventional methods: the combined result of the two effects is to ensure that the different components of the mixture diffuse in opposite directions, leading to high degree of separation. In contrast, traditional methods of separation drive both of the components in the same direction but at different rates. For example, in distillation, the vapor pressure of both components typically increase on heating. Or, an increase in concentration gradient may lead to higher self-diffusivities of both of the species. Consequently, the separation factor is limited by the differential rate of the various components. More importantly, at a practical level, the present method achieves separations at microscopic length scales, as compared to macroscopic length scales in conventional methods, because the basic effects giving raise to the separation operate at nano length scales.

The energy cost associated with the present method is expected to be significantly lower than that in the traditional methods. The hot spot required in the present method will add to the energy cost. However, the nano lengths at which separation is achieved implies that the number of hot spots to be maintained are only few. On the other hand, the lower activation energy⁸ of the guest particle in the anomalous regime ensures that self-diffusivities of reasonable magnitude exist, even at lower temperatures, obviating the need to maintain high temperatures to drive the components. Most of the energy cost in conventional methods of separation is due to this. The energy saved as compared to conventional methods is large ($= C_p \Delta T$ per mole) because it is directly proportional to the mass mixture to be separated. The energy cost in this case is proportional to the amount of gas that is to be separated and is, therefore, an extensive property.

While the present exercise illustrates the combined use of blow torch and levitation effect in the context of separation of mixtures, the concept is clearly more general and should find application in several situations, particularly in biological separations as well as processes. The levitation effect suggests that, if the channel dimension through which the ions diffuse is about the size of the ion, then the activation energy for diffusion is lowest.⁸ We are presently working on ion diffusion across biomembranes to make the above suggestions more concrete.

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