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The FJO thermal diffusion column theory and the thermal diffusion factor

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Abstract. It is shown that by proper choice of a reference temperature in the theoretical expression for the separation factor for a thermal diffusion column, the separation factor may be made to depend on the potential model and the interaction parameters solely through the thermal diffusion factor, the other terms in the expression becoming independent of the model and parameters.

The standard rigorous FJO theory which describes the operation of the thermal diffusion column gives the expression for the reduced logarithm of the maximum separation factor in the steady state as

$$\ln \bar{Q}_0{}^* = \frac{(70)^{1/2}}{20} \frac{L}{r_1} (\alpha_0)_1 \frac{h'}{(\kappa_c{}'\kappa_d{}')^{1/2}} \tag{1}$$

where all the quoted quantities keep their usual meaning (Jones and Furry 1946).

The subscript 1 appearing in this expression refers to the arbitrary choice of the cold-wall temperature as a reference (Furry and Jones 1946, Saxena and Raman 1962).

In this way, and for any potential model, expression (1) takes the functional form

$$\ln \bar{Q}_0{}^* = \alpha_0(T_1, \epsilon/\kappa) F_1(r_1, r_2, T_1, T_2, \epsilon/\kappa). \tag{2}$$

It is not possible to use this expression as a means of determining $(\alpha_0)_1$ from a measured value of $\ln/\bar{Q}_0{}^*$ because the unknown interaction parameter ϵ/κ enters into the shape factors combination F_1, as well as into $(\alpha_0)_1$.

The purpose of this short paper is to show that this inconvenience in the rigorous FJO theory can be obviated by choosing a suitable temperature reference.

Any other choice of temperature reference $T_1 < T_K < T_2$ would, in principle, yield the same functional dependence as (2), but with the thermal diffusion factor and combination of shape factors referring to this new temperature.

What we are interested in is to find out if a T_s exists such as to fulfill the condition

$$\left\{\frac{\partial F_s}{\partial(\epsilon/\kappa)}\right\}_{r_1, r_2, T_1, T_2} = 0. \tag{3}$$

The analytical procedure if it is possible seems extremely tedious, so we therefore proceed to carry out the calculations numerically.

For definiteness, a hot-wire type column (Hidalgo *et al.* 1970) is used with the geometrical characteristics $r_2 = 0{\cdot}02$ cm, $r_1 = 0{\cdot}6$ cm, $L = 119$ cm. For simplicity a two-parameter 'realistic' model such as the *L–J* (12–6) (Hirschfelder *et al.* 1954) is adopted. The procedure is as follows.

(i) Any value of ϵ/κ is taken.

(ii) The $\ln \bar{Q}_0{}^*$ is calculated at fixed working temperatures T_1, T_2.

(iii) From (2) and by dividing the calculated value of ln $\tilde{Q}_0{}^*$ by the (α_0) values ranging from $T_1{}^*$ to $T_2{}^*$, F_k as a function of T_2 is obtained.

(iv) New wide apart values $(\epsilon/\kappa)_2$, $(\epsilon/\kappa)_3$ ..., are taken and the procedure is repeated.

The trend of the different F_k so obtained as functions of temperature and ϵ/κ is plotted in figure 1 for any two particular working temperatures T_1, T_2 available in hot-wire columns. It can be realized that condition (3) is wholly fulfilled by $T_k = T_s$.

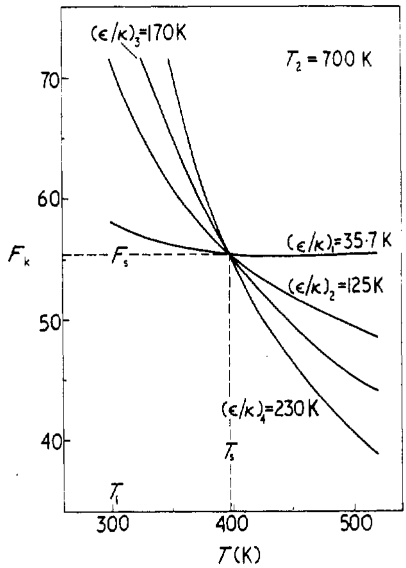

Figure 1. The trend of the F_k function against T ($T_1 < T < T_2$), for different ϵ/κ when column temperatures are T_1 = 301 K and T_2 = 700 K. The *L–J* (12–6) potential model is used.

In table 1 values of F_s and T_s at different T_2, together with their standard errors, are stated. Conclusion: When the temperature reference T_s is taken, the combination

Table 1. The F_s and T_s values for a hot-wire type column (Hidalgo *et al.* 1970) at different T_2 (T_1 = 301 K). The potential model *L–J* (12–6) has been used

T_2 (K)	F_s	T_s
400	15·75 ±0·01	327·7 ±0·5
500	30·31 ±0·04	353·0 ±0.6
600	43·50 ±0·02	377·5 ±0·4
700	55·60 ±0·08	400·3 ±0·7
800	66·6 ±0·2	422·2 ±0·9
900	76·6 ±0·2	443·0 ±2·0
1000	85·9 ±0·3	463·0 ±2·0

of shape factors F_s does not depend on the interaction parameters, i.e. the factor F_s is a constant characteristic of the installation at fixed T_1, T_2.

Hence the expression for $\ln \bar{Q}_0{}^*$ may be turned out in the more convenient form:

$$\ln \bar{Q}_0{}^* = \alpha_0(\epsilon/\kappa, T_s)F_s(T_1, T_2, r_1, r_2)$$

which would allow us to determine $(\alpha_0)_s$ evaluated at an intermediate temperature, $T_1 < T_s < T_2$, without previously fixing the interaction (ϵ/κ).

To judge the influence of the interaction model on F_s and T_s the computations have been repeated using different types of potential models. The *L–J* (75–6) (Klein and Smith 1968) and *L–J* (8–4) (Jones 1941) have been selected from among the 'realistics' as they yield predictions, for the transport properties, drastically different from each other and from the *L–J* (12–6) model. An 'unrealistic' model such as the rigid spheres (α_0 = constant, $\Omega^{*(i,j)} = 1$) has also been tried, in order to carry out a more severe test.

In table 2, the F_s and T_s mean values and their corresponding standard errors, for all models tried and for different T_2, are outlined. Calculations have been performed with the ϵ/κ values stated in figure 1. Tabulations for $\Omega^{*(1,1)}$, $\Omega^{*(2,2)}$ and α_0 were not used directly, but a previous 'smoothing' was performed by means of polynomial fitting. Conclusion: The combination of shape factors F_s and the temperature reference T_s do not depend on the potential model used to describe the gas.

Table 2. Mean values for F_s and T_s obtained for the potential models *L–J* (8–4), *L–J* (12–6), *L–J* (75–6) and rigid spheres at different T_2 (T_1 = 301 K)

T_2(K)	F_s	T_s
400	15·68 ± 0·03	329 ± 2
500	30·10 ± 0·12	356 ± 3
600	43·2 ± 0·2	381 ± 3
700	55·2 ± 0·3	404 ± 4
800	66·1 ± 0·3	425 ± 4
900	76·1 ± 0·4	446 ± 4
1000	85·4 ± 0·4	466 ± 4

From this it is seen that, from a theoretical point of view, the column may be used as a prominent technique to determine $(\alpha_0)_s$, with the advantage over other techniques that the temperature at which the thermal diffusion factor comes out is accurately known, as it is solely a function of the geometry and working temperatures of the installation.

It is shown that, by proper choice of a reference temperature in the theoretical expression for the separation factor for a thermal diffusion column, the separation factor may be made to depend on the potential model and the interaction parameters solely through the thermal diffusion factor, the other terms in the expression becoming independent of the model and parameters.

The experimental consequences of the above quoted results require basically good theoretical–experimental agreement. These aspects and more details relating to this paper are to be published.

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