

Erratum: “The carrier gas pressure effect in a laminar flow diffusion chamber, homogeneous nucleation of *n*-butanol in helium” [J. Chem. Phys. 124, 224304 (2006)]

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A mistake has been found while cross-checking the computer code of a mathematical model¹ of the laminar flow diffusion chamber (LFDC) against the implementation of the same model under a CFD code FLUENT. The mathematical model describes a coupled mass and heat transfer inside the LFDC, and its solution provides (at particular boundary conditions in a steady state) profiles of temperature and vapor concentration in axial and radial directions.

The mistake resided in the implementation of the heat capacity mixing rule for ideal vapor-gas mixture. The pure components' heat capacities in the code are defined in units of $\text{J} \times \text{kg}^{-1} \times \text{K}^{-1}$, because mass fractions together with a mass flow rate are used throughout the code when mass transfer is calculated. In our erroneous implementation, the heat capacity of a mixture was calculated as a mole fraction weighted average instead of a mass fraction weighted average. This error has been fixed and the experimental results published in Hyvärinen *et al.*² Tables I–III have been recalculated.

The implementation of the corrected code decreases the nucleation temperature T_n , and increases the saturation ratio S_n at the nucleation rate maximum, see Table I. The maximum change in nucleation temperature is -0.41 K indicating that the results may still be considered isothermal. Changes in experimental nucleation rate maximum J_{exp} are minute. While values given in Table I can be used to correct for Tables I–III in Ref. 2, the corrected data in tabulated form

can be also obtained through the EPAPS service.³

Because the change in saturation ratio is dependent on pressure, the reported carrier gas pressure effect changes. This can be seen in Fig. 1, where the measured isotherms are illustrated. The previously observed negative effect (decrease of nucleation rate with increasing pressure) disappears. A closer inspection reveals that at temperatures 270 and 265 K even a weak positive effect is observed, although less than one order of magnitude.

Figure 7 and Table IV in the original publication² presented the nucleation rates as a function of total pressure at constant temperature and saturation ratio. As saturation ratio in the experiments was adjusted according to results obtained from the mathematical model, the apparent negative effect in Fig. 7 of the original paper now seems to appear due to saturation ratio decreasing with the increasing pressure.

The molecular content of critical clusters is smaller with the recalculated isotherms. The average ratio of the experimental n_{exp}^* and that calculated from the Kelvin equation n_{Kelvin}^* presented in Fig. 8 of the original paper, is now 0.85. As a function of pressure, the trend remains the same as before. Measurements made at 50 kPa still yield the highest critical cluster sizes.

As a conclusion, the negative pressure effect observed previously with *n*-butanol+helium in a laminar flow diffusion chamber practically disappeared after we corrected the mistake found in the implementation of the mathematical

TABLE I. The difference between the recalculated and previously published (Ref. 2) average nucleation temperatures ΔT and saturation ratios ΔS .

ΔT	50 kPa	100 kPa	210 kPa	ΔS	50 kPa	100 kPa	210 kPa
265 K	-0.19	-0.1	-0.05	265 K	0.31	0.14	0.14
270 K	-0.24	-0.12	-0.03	270 K	0.36	0.17	0.07
275 K	-0.31	-0.15	-0.08	275 K	0.46	0.12	0.09
280 K	-0.41	-0.23	-0.09	280 K	0.52	0.35	0.21

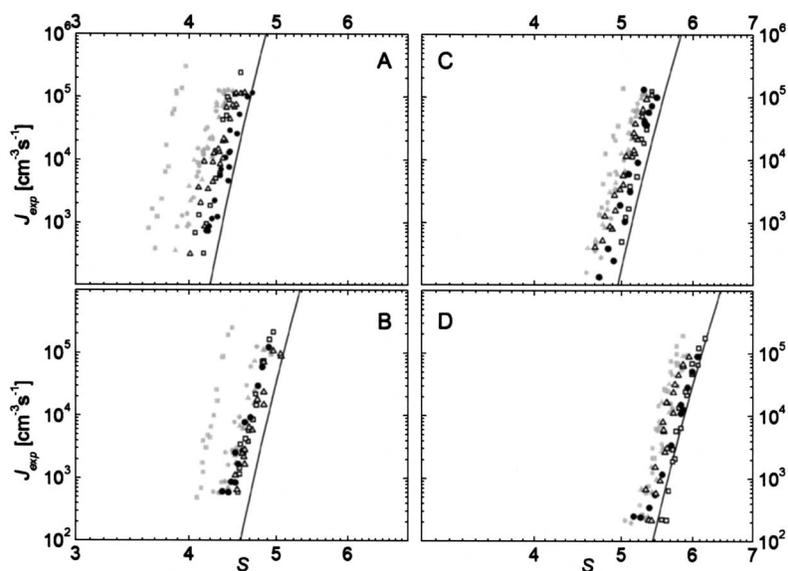


FIG. 1. The experimental nucleation rates J_{exp} as a function of saturation ratio S of n -butanol. Squares are measurements at 50 kPa data, circles are measurements at 100 kPa and triangles are measurements at 210 kPa. Grey symbols are the previously measured data, and filled and open symbols are the recalculated data. (A) is isotherm 280 K, (B) is isotherm 275 K, (C) is isotherm 270 K, (D) is isotherm 265 K. Solid lines are predictions from the classical nucleation theory.

model. A slight positive effect is observed at 270 and 265 K, but the effect resides inside the limits of experimental uncertainty presented in the original paper.²

¹H. Lihavainen and Y. Viisanen, *J. Phys. Chem. B* **105**, 11619 (2001).

²A.-P. Hyvärinen, D. Brus, V. Ždímal, J. Smolík, M. Kulmala, Y. Viisanen, and H. Lihavainen, *J. Chem. Phys.* **124**, 224304 (2006).

³See EPAPS Document No. E-JCPSA6-128-014808 for recalculated data. This document can be reached through a direct link in the online article's HTML reference section or via the EPAPS homepage (<http://www.aip.org/pubservs/epaps.html>).