Data Article

Dataset on the carbon dioxide, methane and nitrogen high-pressure sorption properties of South African bituminous coals

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A B S T R A C T

The dataset presented in this article supplements the result and information published in the report “The carbon dioxide, methane and nitrogen high-pressure sorption properties of South African bituminous coals” (Okolo et al., 2019). Four run of mine coal samples from selected underground coal mines from the Highveld, Witbank, and Tshipise-Pafuri coalfields of South Africa were used for the study. The CO2, CH4, and N2 sorption data were acquired from an in-house built high-pressure gravimetric sorption system (HPGSS) at the CSIRO Energy, North Ryde, Australia; at an isothermal temperature of 55 °C, in the pressure range: 0.1–16 MPa. The resulting excess sorption isotherm data were fitted to the modified Dubinin-Radushkevich isotherm model (M-DR) and a new Dubinin-Radushkevich — Henry law hybrid isotherm model (DR-HH). The dataset provided in this article, apart from being informative will be useful for comparison with available and future data and for testing other sorption isotherm models developed by other investigators in the area of CO2 storage in geological media, especially coal seams.

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1. Data

The research dataset presented in this data report supplements the result and information published in the International Journal of Coal Geology [1], and consists of 5 tables, 1 figure, and 3 graphs (total 4 figures). Fig. 1 shows a not-drawn-to-scale schematic of the HPGSS adapted from Day et al. [4], while Table 1 presents the experimental factors, including sample mass and density. In Table 2, the systematically analysed data from the HPGSS for the 3 adsorbate gases (CO2, CH4, and N2) are presented. Figs. 2 and 3 show the experimental sorption isotherms of the samples for the three gases, and further compares the resulting isotherms with regards to the 4 coals, as well the 3 adsorbate gases. In Tables 3–5, the M-DR and DR-HH excess sorption isotherm model fittings data are provided for the 3 gases, while Fig. 4 depicts the graphical representation of the M-DR and DR-HH excess sorption isotherm fittings to the experimental excess sorption data of the coal samples for all three adsorbate gases (CO2, CH4, and N2) in 2–D rendering.

2. Experimental design, materials, and methods

The HPGSS and the experimental procedure has been previously described in details [1,2,4–6]. Briefly, the prepared samples were dried and degassed in a vacuum oven at 60 °C for 2 weeks prior to the sorption experiments. After this, the samples were weighed and loaded into the sample cells, and placed in the isothermal oven environment maintained at the experimental temperature of 55 °C. Further degassing was continued on the samples in the sample cells in the oven at < 0.5 mbar for another 24 hr. The sorption experiments were started on the samples by a stepwise pressure increment from 0.1 MPa to 16 MPa. It should be noted the density of the samples were measured on a Quantachrome Instruments Ultrapyc 1200e gas pycnometer before drying and degassing. The sorption experiments on the samples were conducted in the order: firstly, CO2, then CH4, and lastly, N2. After
Fig. 1. Schematic diagram of the high-pressure gravimetric sorption system (HPGSS) (Adapted from Day et al. [4]; Not drawn to scale).

Table 1
Experimental factors.

| Sample ID/parameters | DEN     | OGS     | FOZ     | TKD     |
|----------------------|---------|---------|---------|---------|
| Sample weight (g)    | 225.29  | 229.04  | 220.48  | 225.45  |
| Density (kg m\(^{-3}\)) | 1685.4  | 1574.6  | 1533.3  | 1487.6  |
| Sample cell location | Cell #1 | Cell #2 | Cell #3 | Cell #4 |
| Isothermal temperature (°C) | 55 °C   |         |         |         |

Table 2
CO\(_2\), CH\(_4\), and N\(_2\) excess sorption isotherm data of the coal samples.

| Pressure, P (MPa) | Gas density, \(\rho_g\) (kg m\(^{-3}\)) | DEN     | OGS     | FOZ     | TKD     |
|-------------------|----------------------------------------|---------|---------|---------|---------|
| 0.1052            | 1.7036                                 | 6.0806  | 6.9664  | 7.2911  | 4.6445  |
| 0.2200            | 3.5776                                 | 10.7999 | 11.7390 | 12.5281 | 8.4804  |
| 0.4391            | 7.1986                                 | 16.2837 | 17.1022 | 18.4398 | 13.5907 |
| 1.0537            | 17.6856                                | 24.5218 | 24.7386 | 27.3530 | 20.0485 |
| 2.0561            | 35.9626                                | 31.6399 | 31.2187 | 35.2323 | 25.2720 |
| 4.1348            | 79.8852                                | 38.9013 | 37.9850 | 43.8449 | 30.4186 |
| 6.1843            | 135.4973                               | 41.9272 | 41.1873 | 48.2612 | 32.6679 |
| 8.0911            | 207.9895                               | 42.1776 | 42.4067 | 50.1199 | 33.2439 |
| 10.1733           | 339.8949                               | 38.6201 | 40.9607 | 48.9972 | 32.4170 |
| 12.1105           | 513.7378                               | 33.7485 | 39.1124 | 47.0691 | 31.4816 |
| 14.2367           | 628.0571                               | 30.1006 | 37.9188 | 45.6193 | 31.0692 |
| 16.2377           | 687.2398                               | 28.2556 | 37.2927 | 44.8803 | 30.6997 |
Table 2 (continued)

Methane (CH₄) excess sorption, $Q_{exc}$ (kg t⁻¹ (db))

| Pressure, $P$ (MPa) | Gas density, $ρ_g$ (kg m⁻³) | DEN | OGS | FOZ | TKD |
|---------------------|-----------------------------|-----|-----|-----|-----|
| 0.1132              | 0.6667                      | 0.4626 | 0.5353 | 0.5931 | 0.1540 |
| 0.2315              | 1.3654                      | 1.1887 | 1.4192 | 1.4724 | 1.1590 |
| 0.4750              | 2.8093                      | 2.4788 | 2.5649 | 2.8562 | 1.1789 |
| 1.0787              | 6.4262                      | 3.7639 | 3.9360 | 4.3866 | 2.8467 |
| 2.0661              | 12.4510                     | 5.1266 | 5.3528 | 6.0100 | 4.6008 |
| 4.0324              | 24.8426                     | 7.0223 | 7.3055 | 8.3525 | 6.2769 |
| 6.1552              | 38.7681                     | 7.9628 | 8.3468 | 9.6534 | 6.8408 |
| 8.1611              | 52.3585                     | 8.4773 | 8.9687 | 10.5230 | 7.3252 |
| 10.1568             | 66.1680                     | 8.7613 | 9.4076 | 11.0862 | 7.5526 |
| 12.1650             | 80.1984                     | 8.9539 | 9.8511 | 11.5986 | 7.8396 |
| 14.1102             | 93.7198                     | 8.8566 | 9.8813 | 11.7484 | 8.3331 |
| 16.1754             | 107.8090                    | 8.9885 | 10.3417 | 12.2172 | 8.8618 |

Nitrogen (N₂) excess sorption, $Q_{exc}$ (kg t⁻¹ (db))

| Pressure, $P$ (MPa) | Gas density, $ρ_g$ (kg m⁻³) | DEN | OGS | FOZ | TKD |
|---------------------|-----------------------------|-----|-----|-----|-----|
| 0.1684              | 1.7289                      | 0.2238 | 0.2612 | 0.3178 | 0.4433 |
| 0.3188              | 3.2734                      | 0.7251 | 0.8487 | 0.9541 | 0.7732 |
| 0.6249              | 6.4174                      | 1.0927 | 1.3153 | 1.4904 | 1.2927 |
| 1.1028              | 11.3211                     | 2.1631 | 2.4872 | 2.7902 | 2.1388 |
| 2.0654              | 21.1906                     | 3.4196 | 3.7688 | 4.3234 | 3.2797 |
| 4.0553              | 41.5046                     | 5.3570 | 6.0511 | 6.9245 | 5.5327 |
| 6.0860              | 62.0460                     | 6.5543 | 7.4166 | 8.7065 | 6.3771 |
| 8.1248              | 82.3925                     | 7.4455 | 8.6282 | 9.8850 | 7.1077 |
| 10.1292             | 102.0160                    | 7.9476 | 9.4314 | 10.8222 | 7.9509 |
| 12.1536             | 121.4200                    | 8.5399 | 10.3162 | 11.9149 | 8.8667 |
| 14.1483             | 140.0341                    | 8.9066 | 10.8615 | 12.6648 | 9.0379 |
| 16.1510             | 158.2013                    | 9.0753 | 10.7315 | 13.2479 | 9.2338 |

Fig. 2. Comparison of the CO₂, CH₄, and N₂ excess sorption isotherms for each sample.
Fig. 3. Comparison of the CO₂, CH₄, and N₂ excess sorption isotherms of the samples with respect to the adsorbate gases.

Table 3
M-DR and DR-HH excess sorption isotherm model fittings data for CO₂ experimental excess sorption data.

| Pressure, P (MPa) | Gas density, \( \rho_g \) (kgm\(^{-3}\)) | Experimental excess sorption, \( Q_{exc} \) (kg t\(^{-1}\)) (db) | M-DR fitting (kg t\(^{-1}\)) (db) | DR-HH fitting (kg t\(^{-1}\)) (db) | \( Q_{exc} \) (kg t\(^{-1}\)) (db) | M-DR fitting (kg t\(^{-1}\)) (db) | DR-HH fitting (kg t\(^{-1}\)) (db) |
|------------------|---------------------------------|--------------------------------------------------|-------------------------------|-----------------------------------|-----------------------------|-------------------------------|-----------------------------------|
| 0.1052           | 1.7036                          | 6.0806                                          | 5.5292                        | 7.0842                            | 6.9664                      | 4.3963                        | 8.0316                            |
| 0.2200           | 3.5776                          | 10.7999                                         | 9.4612                        | 11.1356                           | 11.7390                     | 8.0676                        | 12.6018                           |
| 0.4391           | 7.1986                          | 16.2837                                         | 14.7451                       | 16.1866                           | 17.1022                     | 13.3247                       | 16.8980                           |
| 1.0537           | 17.6856                         | 24.5218                                         | 23.7851                       | 24.2453                           | 24.7386                     | 22.9005                       | 24.3754                           |
| 2.0561           | 35.9626                         | 31.6399                                         | 32.0643                       | 31.2489                           | 31.2187                     | 32.1680                       | 30.7866                           |
| 4.1348           | 79.8852                         | 38.9013                                         | 40.7069                       | 38.3924                           | 37.9850                     | 42.3714                       | 37.5065                           |
| 6.1843           | 135.4973                        | 41.9272                                         | 44.3324                       | 41.5152                           | 41.1873                     | 47.0264                       | 40.8765                           |
| 8.0911           | 207.9895                        | 42.1776                                         | 44.7251                       | 42.2269                           | 42.4067                     | 48.0223                       | 42.4218                           |
| 10.1733          | 339.8949                        | 38.6201                                         | 40.6563                       | 39.9134                           | 40.9607                     | 44.1092                       | 42.2191                           |
| 12.1105          | 513.7378                        | 33.7485                                         | 31.7767                       | 34.2606                           | 39.1124                     | 34.6763                       | 39.7987                           |
| 14.2367          | 628.0571                        | 30.1006                                         | 25.0701                       | 29.9087                           | 37.9188                     | 27.4088                       | 37.6858                           |
| 16.2377          | 687.2398                        | 28.2556                                         | 21.4643                       | 27.5584                           | 37.2927                     | 23.4813                       | 36.5122                           |

| Pressure, P (MPa) | Gas density, \( \rho_g \) (kgm\(^{-3}\)) | Experimental excess sorption, \( Q_{exc} \) (kg t\(^{-1}\)) (db) | M-DR fitting (kg t\(^{-1}\)) (db) | DR-HH fitting (kg t\(^{-1}\)) (db) | \( Q_{exc} \) (kg t\(^{-1}\)) (db) | M-DR fitting (kg t\(^{-1}\)) (db) | DR-HH fitting (kg t\(^{-1}\)) (db) |
|------------------|---------------------------------|--------------------------------------------------|-------------------------------|-----------------------------------|-----------------------------|-------------------------------|-----------------------------------|
| 0.1052           | 1.7036                          | 7.2911                                          | 3.9272                        | 8.1898                            | 4.6445                      | 3.3059                        | 6.2127                            |
| 0.2200           | 3.5776                          | 12.5281                                         | 7.7049                        | 12.7049                           | 8.4804                      | 6.1577                        | 9.3805                            |
| 0.4391           | 7.1986                          | 18.4398                                         | 13.4515                       | 18.2864                           | 13.3907                     | 10.2965                       | 13.2017                           |
| 1.0537           | 17.6856                         | 27.3530                                         | 24.5622                       | 27.1749                           | 20.0485                     | 17.9364                       | 19.1438                           |
| 2.0561           | 35.9626                         | 35.2323                                         | 35.8854                       | 35.0037                           | 25.2720                     | 25.4165                       | 24.2717                           |
| 4.1348           | 79.8852                         | 43.8449                                         | 48.9620                       | 43.4222                           | 30.4186                     | 33.7418                       | 29.6993                           |
| 6.1843           | 135.4973                        | 48.2612                                         | 55.3324                       | 47.8210                           | 32.6679                     | 37.5997                       | 32.4777                           |
| 8.0911           | 207.9895                        | 50.1199                                         | 57.1634                       | 50.0444                           | 33.2439                     | 38.4953                       | 33.8250                           |
| 10.1733          | 339.8949                        | 48.9972                                         | 53.0289                       | 50.1941                           | 32.4170                     | 35.4366                       | 33.8648                           |
| 12.1105          | 513.7378                        | 47.0691                                         | 41.9207                       | 47.7231                           | 31.4816                     | 27.8929                       | 32.1928                           |
| 14.2367          | 628.0571                        | 45.6193                                         | 33.1939                       | 45.4365                           | 31.0692                     | 22.0558                       | 30.6755                           |
| 16.2377          | 687.2398                        | 44.8803                                         | 28.4547                       | 44.1512                           | 30.6997                     | 18.8979                       | 29.8260                           |
Table 4
M-DR and DR-HH excess sorption isotherm model fittings data for CH₄ experimental excess sorption data.

| Pressure, P (MPa) | Gas density, \( r_g \) (kg m\(^{-3} \)) | DEN (CH₄) | M-DR fitting, \( Q_{exc}(kg \cdot m^{-1}) \) (db) | DR-HH fitting, \( Q_{exc}(kg \cdot m^{-1}) \) (db) | OGS (CH₄) | Experimental excess sorption, \( Q_{exc}(kg \cdot m^{-1}) \) (db) | M-DR fitting, \( Q_{exc}(kg \cdot m^{-1}) \) (db) | DR-HH fitting, \( Q_{exc}(kg \cdot m^{-1}) \) (db) |
|------------------|----------------------------------------|------------|---------------------------------------------|---------------------------------------------|------------|-------------------------------------------------|---------------------------------------------|---------------------------------------------|
| 0.1132           | 0.6667                                 | 0.4626     | 0.5796                                      | 0.6997                                      | 0.5353     | 0.5171                                           | 0.8068                                      | 0.8191                                      |
| 0.2315           | 1.3654                                 | 1.1887     | 1.1364                                      | 1.2883                                      | 1.4192     | 1.0622                                           | 1.4314                                      | 1.3914                                      |
| 0.4750           | 2.8093                                 | 2.4788     | 2.0576                                      | 2.2097                                      | 2.5649     | 2.0044                                           | 2.3795                                      | 2.3795                                      |
| 1.0787           | 6.4262                                 | 3.7639     | 3.6542                                      | 3.7324                                      | 3.9360     | 3.7064                                           | 3.9134                                      | 3.9134                                      |
| 2.0661           | 12.4510                                | 5.1266     | 5.3041                                      | 5.2609                                      | 5.3528     | 5.5266                                           | 5.4489                                      | 5.4489                                      |
| 4.0324           | 24.8426                                | 7.0223     | 7.1433                                      | 6.9632                                      | 7.3055     | 7.6163                                           | 7.2103                                      | 7.2103                                      |
| 6.1552           | 38.7681                                | 7.9628     | 8.1640                                      | 7.9513                                      | 8.3468     | 8.8102                                           | 8.3191                                      | 8.3191                                      |
| 8.1611           | 52.3585                                | 8.4773     | 8.6559                                      | 8.4835                                      | 8.9687     | 9.4060                                           | 9.0021                                      | 9.0021                                      |
| 10.1568          | 66.1680                                | 8.7613     | 8.8659                                      | 8.7802                                      | 9.4076     | 9.6796                                           | 9.4731                                      | 9.4731                                      |
| 12.1650          | 80.1984                                | 8.9539     | 8.8884                                      | 8.9229                                      | 9.8511     | 9.7375                                           | 9.8075                                      | 9.8075                                      |
| 14.1102          | 93.7198                                | 8.8566     | 8.7857                                      | 8.9576                                      | 9.8813     | 9.6488                                           | 10.0370                                     | 10.0370                                     |
| 16.1754          | 107.8090                               | 8.9885     | 8.5857                                      | 8.9175                                      | 10.3417    | 9.4481                                           | 10.0767                                     | 10.0767                                     |

Table 5
M-DR and DR-HH excess sorption isotherm model fittings data for N₂ experimental excess sorption data.

| Pressure, P (MPa) | Gas density, \( r_g \) (kg m\(^{-3} \)) | DEN (N₂) | M-DR fitting, \( Q_{exc}(kg \cdot m^{-1}) \) (db) | DR-HH fitting, \( Q_{exc}(kg \cdot m^{-1}) \) (db) | OGS (N₂) | Experimental excess sorption, \( Q_{exc}(kg \cdot m^{-1}) \) (db) | M-DR fitting, \( Q_{exc}(kg \cdot m^{-1}) \) (db) | DR-HH fitting, \( Q_{exc}(kg \cdot m^{-1}) \) (db) |
|------------------|----------------------------------------|------------|---------------------------------------------|---------------------------------------------|------------|-------------------------------------------------|---------------------------------------------|---------------------------------------------|
| 0.1132           | 0.6667                                 | 0.5931     | 0.4990                                      | 0.8043                                      | 0.1540     | 0.3195                                           | 0.4817                                      | 0.4817                                      |
| 0.2315           | 1.3654                                 | 1.4724     | 1.0731                                      | 1.5271                                      | 1.1590     | 0.7027                                           | 0.9275                                      | 0.9275                                      |
| 0.4750           | 2.8093                                 | 2.8562     | 2.1086                                      | 2.5945                                      | 1.1789     | 1.4084                                           | 1.6577                                      | 1.6577                                      |
| 1.0787           | 6.4262                                 | 4.3866     | 4.0567                                      | 4.3615                                      | 2.8467     | 2.7627                                           | 2.9240                                      | 2.9240                                      |
| 2.0661           | 12.4510                                | 6.0100     | 6.2109                                      | 6.1676                                      | 4.6008     | 4.2846                                           | 4.2595                                      | 4.2595                                      |
| 4.0324           | 24.8426                                | 8.3525     | 8.7547                                      | 8.2830                                      | 6.2769     | 6.1065                                           | 5.8426                                      | 5.8426                                      |
| 6.1552           | 38.7681                                | 9.6534     | 10.2477                                     | 9.6456                                      | 6.8408     | 7.1984                                           | 6.8499                                      | 6.8499                                      |
| 8.1611           | 52.3585                                | 10.5230    | 11.0153                                     | 10.5049                                     | 7.3252     | 7.7536                                           | 7.4645                                      | 7.4645                                      |
| 10.1568          | 66.1680                                | 11.0862    | 11.3883                                     | 11.1355                                     | 7.5526     | 8.0343                                           | 7.8785                                      | 7.8785                                      |
| 12.1650          | 80.1984                                | 11.5986    | 11.4949                                     | 11.5601                                     | 7.8396     | 8.1228                                           | 8.1609                                      | 8.1609                                      |
| 14.1102          | 93.7198                                | 11.7484    | 11.4180                                     | 11.8797                                     | 8.3331     | 8.0781                                           | 8.3433                                      | 8.3433                                      |
| 16.1754          | 107.8090                               | 12.2172    | 11.2024                                     | 12.1304                                     | 8.8618     | 7.9331                                           | 8.4662                                      | 8.4662                                      |
each adsorbate gas exposure to the samples, the samples were degassed for a minimum of 48 hrs before the next gas is sorbed onto the sample. The HPGSS can hold four sample cells simultaneously, thus, gas sorption on all four samples were done at the same time.

Data logging from the HPGSS is automated with the aid of data logging hardware and software coupled to the system. Data logged from the facility include, mass gain, real time, pressure, and temperature. The resulting raw data was filtered to remove data acquired at non-equilibrium state. Only equilibrium data at constant mass over a long time (usually ≥ 8 hr) were collected and analysed. The excess sorbed amount was calculated using Equation (1) [1,2,7]:

Table 5 (continued)

| Pressure, $P$ (MPa) | Gas density, $\rho_g$ (kgm$^{-3}$) | DEN ($N_2$) | OGS ($N_2$) |
|---------------------|-----------------------------------|-------------|-------------|
|                     |                                   | Experimental excess sorption, $Q_{exc}$ (kgt$^{-1}$) (db) | M-DR fitting ($kgt^{-1}$) (db) | DR-HH fitting ($kgt^{-1}$) (db) | Experimental excess sorption, $Q_{exc}$ (kgt$^{-1}$) (db) | M-DR fitting ($kgt^{-1}$) (db) | DR-HH fitting ($kgt^{-1}$) (db) |
| 0.1684              | 1.7289                            | 0.3178      | 0.1919      | 0.4116      | 0.4433      | 0.2029      | 0.3491      |
| 0.3188              | 3.2734                            | 0.9541      | 0.4930      | 0.8366      | 0.7732      | 0.4792      | 0.6963      |
| 0.6249              | 6.4174                            | 1.4904      | 1.1872      | 1.6352      | 1.2927      | 1.0663      | 1.3327      |
| 1.1028              | 11.3211                           | 2.7902      | 2.2667      | 2.7010      | 2.1388      | 1.9204      | 2.1613      |
| 2.0654              | 21.1906                           | 4.3234      | 4.1751      | 4.3939      | 3.2797      | 3.3452      | 3.4417      |
| 4.0553              | 41.5046                           | 6.9245      | 7.0762      | 6.8485      | 5.5327      | 5.3944      | 5.2285      |
| 6.0860              | 62.0460                           | 8.7065      | 9.0554      | 8.6017      | 6.3771      | 6.7344      | 6.4497      |
| 8.1248              | 82.3925                           | 9.8850      | 10.4074     | 9.9407      | 7.1077      | 7.6230      | 7.3447      |
| 10.1292             | 102.0160                          | 10.8222     | 11.3142     | 10.9931     | 7.9509      | 8.2028      | 8.0204      |
| 12.1536             | 121.4200                          | 11.9149     | 11.9299     | 11.8735     | 8.8667      | 8.5841      | 8.5636      |
| 14.1483             | 140.0341                          | 12.6648     | 12.3199     | 12.6078     | 9.0379      | 8.8146      | 8.9989      |
| 16.1510             | 158.2013                          | 13.2479     | 12.5508     | 13.2444     | 9.2338      | 8.9397      | 9.3618      |

Fig. 4. M-DR and DR-HH isotherm model fittings to the experimental (a) CO$_2$, (b) CH$_4$, and (c) N$_2$ experimental excess sorption data of the coal samples.
\[ Q_{\text{exc}} = M_{\text{mea}} - (V_{\text{cell}} - V_{\text{sample}}) \rho_g \]  

(1)

\[ Q_{\text{exc}} = Q_0 \left(1 - \frac{\rho_g}{\rho_a}\right) \exp \left[-D \left(\ln \frac{\rho_a}{\rho_g}\right)^2\right] \]  

(2)

\[ Q_{\text{exc}} = Q_0 \left(1 - \frac{\rho_g}{\rho_a}\right) \exp \left[-D \left(\ln \frac{\rho_a}{\rho_g}\right)^2\right] + k \rho_g \]  

(3)

Where, \( Q_{\text{exc}} \), is the excess (Gibbs') sorption (kg); \( M_{\text{mea}} \), is the measured mass of adsorbate at a given pressure (kg); \( V_{\text{cell}} \), is the volume of sample cell (m\(^3\)); \( V_{\text{sample}} \), is the volume of sample (m\(^3\)); \( Q_0 \), is the maximum sorption capacity by weight (kg/tcoal); \( \rho_a \), is the adsorbed phase density (kgm\(^{-3}\)); \( \rho_g \), is the adsorbate gas density (kgm\(^{-3}\)); \( D \), is the affinity constant (\(-\)); \( k \), is the proportionality constant (ml/g).

The maximum sorption capacities of the samples for the 3 gases were determined by fitting the experimental excess sorption data to the M-DR (Equation (2)) and the DR-HH (Equation (3)) excess sorption isotherm models [1,2,7]. Numerical analysis and model fitting was accomplished using the Visual Basic for Application (VBA) macros that were scripted and executed in Microsoft™ Excel 2013.

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**Conflict of interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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