Table 1S. Calculated model parameters and statistical parameters for Henderson-Pabis model

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| T  [°C] | p  [mbar] | Adjustable coefficients | | *R*2 | | AARD [%] | RMSE | | *χ*2 |
|  |  | a | k |  |  | |  |  | |
| 50 | 20 | 96.16 | 0.1311 | 0.9277 | 13.33 | | 5.8062 | 0.1037 | |
| 65 | 92.99 | 0.0689 | 0.9641 | 5.33 | | 3.2037 | 0.0406 | |
| 110 | 89.65 | 0.0398 | 0.9794 | 1.62 | | 1.3607 | 0.0209 | |
| 155 | 86.43 | 0.0497 | 0.9803 | 2.38 | | 1.7355 | 0.0222 | |
| 200 | 82.07 | 0.0187 | 0.9897 | 0.52 | | 0.4371 | 0.0070 | |
| 55 | 20 | 95.15 | 0.1328 | 0.9369 | 12.41 | | 5.3606 | 0.0957 | |
| 65 | 85.42 | 0.0467 | 0.9970 | 0.92 | | 0.6543 | 0.0079 | |
| 110 | 81.39 | 0.0308 | 0.9984 | 0.49 | | 0.3813 | 0.0039 | |
| 155 | 84.11 | 0.0165 | 0.9962 | 0.20 | | 0.1880 | 0.0040 | |
| 200 | 87.15 | 0.0099 | 0.9953 | 0.22 | | 0.2298 | 0.0027 | |
| 60 | 20 | 92.88 | 0.1456 | 0.9527 | 11.17 | | 4.5943 | 0.0851 | |
| 20 | 93.84 | 0.1311 | 0.9421 | 8.58 | | 4.5152 | 0.0982 | |
| 20 | 93.92 | 0.1490 | 0.9402 | 10.58 | | 4.9472 | 0.1075 | |
| 65 | 89.05 | 0.0937 | 0.9840 | 3.75 | | 2.1043 | 0.0339 | |
| 110 | 82.41 | 0.0605 | 0.9978 | 0.75 | | 0.5649 | 0.0084 | |
| 155 | 85.36 | 0.0365 | 0.9966 | 0.60 | | 0.5457 | 0.0072 | |
| 200 | 86.34 | 0.0273 | 0.9982 | 0.45 | | 0.3641 | 0.0040 | |
| 65 | 20 | 92.98 | 0.1861 | 0.9456 | 17.83 | | 5.3701 | 0.1074 | |
| 65 | 85.84 | 0.0876 | 0.9922 | 2.07 | | 1.2505 | 0.0227 | |
| 110 | 84.25 | 0.0636 | 0.9912 | 2.03 | | 1.2900 | 0.0174 | |
| 155 | 79.18 | 0.0545 | 0.9976 | 0.91 | | 0.5877 | 0.0075 | |
| 200 | 84.63 | 0.0314 | 0.9964 | 0.52 | | 0.4686 | 0.0065 | |
| 70 | 20 | 94.68 | 0.1897 | 0.9304 | 18.16 | | 6.0664 | 0.1348 | |
| 65 | 91.04 | 0.1315 | 0.9655 | 8.43 | | 3.7035 | 0.0650 | |
| 110 | 86.18 | 0.0853 | 0.9843 | 3.79 | | 2.0404 | 0.0291 | |
| 155 | 83.47 | 0.0741 | 0.9963 | 1.28 | | 0.8194 | 0.0128 | |
| 200 | 81.92 | 0.0637 | 0.9981 | 0.84 | | 0.5528 | 0.0079 | |

Table 2S. Calculated model parameters and statistical parameters for Modified Henderson-Pabis model

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| T  [°C] | p  [mbar] | Adjustable coefficients | | | | | | *R*2 | AARD [%] | RMSE | *χ*2 |
|  |  | a | k | b | g | c | h |  |  |  |  |
| 50 | 20 | 32.0508 | 0.1311 | 32.0508 | 0.1311 | 32.0508 | 0.1311 | 0.9277 | 13.33 | 5.8062 | 0.1117 |
| 65 | 30.9957 | 0.0689 | 30.9957 | 0.0689 | 30.9957 | 0.0689 | 0.9641 | 5.33 | 3.2037 | 0.0427 |
| 110 | 29.8836 | 0.0398 | 29.8836 | 0.0398 | 29.8835 | 0.0398 | 0.9794 | 1.62 | 1.3607 | 0.0223 |
| 155 | 28.8032 | 0.0497 | 28.7950 | 0.0497 | 28.8247 | 0.0497 | 0.9803 | 2.38 | 1.7355 | 0.0235 |
| 200 | 27.6938 | 0.0455 | 27.6884 | 0.0456 | 27.3875 | -0.0200 | 0.9955 | 0.28 | 0.2901 | 0.0050 |
| 55 | 20 | 31.7110 | 0.1329 | 31.7204 | 0.1329 | 31.7248 | 0.1329 | 0.9369 | 12.41 | 5.3606 | 0.1031 |
| 65 | 28.4750 | 0.0467 | 28.4741 | 0.0467 | 28.4749 | 0.0467 | 0.9970 | 0.92 | 0.6543 | 0.0083 |
| 110 | 27.1312 | 0.0308 | 27.1314 | 0.0308 | 27.1301 | 0.0308 | 0.9984 | 0.49 | 0.3813 | 0.0040 |
| 155 | 28.1267 | 0.0579 | 28.1351 | -0.0004 | 28.1350 | 0.0002 | 0.9981 | 0.14 | 0.1320 | 0.0031 |
| 200 | 29.0286 | 0.0348 | 29.2287 | 0.0003 | 29.2293 | 0.0000 | 0.9973 | 0.18 | 0.1747 | 0.0022 |
| 60 | 20 | 30.9586 | 0.1456 | 30.9586 | 0.1455 | 30.9586 | 0.1455 | 0.9527 | 11.18 | 4.5943 | 0.0919 |
| 20 | 31.2806 | 0.1311 | 31.2827 | 0.1311 | 31.2822 | 0.1312 | 0.9421 | 8.58 | 4.5152 | 0.1075 |
| 20 | 31.3043 | 0.1490 | 31.3044 | 0.1490 | 31.3044 | 0.1490 | 0.9402 | 10.58 | 4.9472 | 0.1178 |
| 65 | 29.6806 | 0.0937 | 29.6852 | 0.0937 | 29.6789 | 0.0937 | 0.9840 | 3.75 | 2.1043 | 0.0363 |
| 110 | 27.4702 | 0.0605 | 27.4720 | 0.0605 | 27.4688 | 0.0605 | 0.9978 | 0.75 | 0.5649 | 0.0090 |
| 155 | 28.5151 | 0.0281 | 28.4893 | 0.0565 | 28.5147 | 0.0281 | 0.9966 | 0.62 | 0.5414 | 0.0075 |
| 200 | 28.7799 | 0.0273 | 28.7794 | 0.0273 | 28.7812 | 0.0274 | 0.9982 | 0.45 | 0.3641 | 0.0042 |
| 65 | 20 | 30.9910 | 0.1861 | 30.9910 | 0.1861 | 30.9910 | 0.1861 | 0.9456 | 17.83 | 5.3701 | 0.1167 |
| 65 | 28.6118 | 0.0876 | 28.6118 | 0.0876 | 28.6118 | 0.0876 | 0.9922 | 2.07 | 1.2505 | 0.0245 |
| 110 | 28.0827 | 0.0636 | 28.0827 | 0.0636 | 28.0827 | 0.0636 | 0.9911 | 2.03 | 1.2900 | 0.0184 |
| 155 | 26.3983 | 0.0545 | 26.4028 | 0.0545 | 26.3757 | 0.0545 | 0.9976 | 0.91 | 0.5877 | 0.0079 |
| 200 | 28.5728 | 0.0155 | 28.1379 | 0.0778 | 28.5905 | 0.0152 | 0.9978 | 0.42 | 0.3691 | 0.0054 |
| 70 | 20 | 31.5564 | 0.1897 | 31.5564 | 0.1897 | 31.5564 | 0.1897 | 0.9304 | 18.16 | 6.0664 | 0.1480 |
| 65 | 30.3492 | 0.1315 | 30.3443 | 0.1315 | 30.3465 | 0.1315 | 0.9655 | 8.43 | 3.7035 | 0.0699 |
| 110 | 28.7255 | 0.0853 | 28.7255 | 0.0853 | 28.7255 | 0.0853 | 0.9843 | 3.79 | 2.0404 | 0.0309 |
| 155 | 27.8234 | 0.0742 | 27.8238 | 0.0741 | 27.8239 | 0.0742 | 0.9963 | 1.28 | 0.8194 | 0.0137 |
| 200 | 27.3067 | 0.0637 | 27.3063 | 0.0637 | 27.3083 | 0.0636 | 0.9981 | 0.84 | 0.5528 | 0.0084 |

Table 3S. Calculated model parameters and statistical parameters for Simplified Fick’s diffusion model

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| T  [°C] | p  [mbar] | Adjustable coefficients | | | *R*2 | AARD [%] | RMSE | *χ*2 |
|  |  | a | c | L |  |  |  |  |
| 50 | 20 | 96.16 | 25.60 | 13.97 | 0.9277 | 13.33 | 5.8062 | 0.1056 |
| 65 | 92.98 | 14.09 | 14.30 | 0.9641 | 5.33 | 3.2037 | 0.0411 |
| 110 | 89.65 | 10.85 | 16.51 | 0.9794 | 1.62 | 1.3607 | 0.0213 |
| 155 | 86.43 | 3.77 | 8.71 | 0.9803 | 2.38 | 1.7355 | 0.0225 |
| 200 | 82.07 | 4.41 | 15.36 | 0.9870 | 0.52 | 0.4371 | 0.0072 |
| 55 | 20 | 95.14 | 23.92 | 13.42 | 0.9370 | 12.42 | 5.3606 | 0.0975 |
| 65 | 85.42 | 16.64 | 18.87 | 0.9970 | 0.92 | 0,6543 | 0,0080 |
| 110 | 81.39 | 5.71 | 13.60 | 0.9940 | 0.47 | 0,5159 | 0,0053 |
| 155 | 84.11 | 3.37 | 14.30 | 0.9962 | 0.20 | 0.1880 | 0.0041 |
| 200 | 87.15 | 1.50 | 12.29 | 0.9953 | 0.22 | 0,2298 | 0,0028 |
| 60 | 20 | 92.88 | 8.16 | 7.49 | 0.9527 | 11.18 | 4.5943 | 0.0867 |
| 20 | 93.84 | 25.40 | 13.92 | 0.9421 | 8.58 | 4.5152 | 0.1003 |
| 20 | 93.92 | 9.43 | 7.96 | 0.9402 | 10.58 | 4.9472 | 0.1099 |
| 65 | 89.05 | 6.86 | 8.56 | 0.9840 | 3.75 | 2.1043 | 0.0345 |
| 110 | 82.41 | 25.81 | 20.65 | 0.9978 | 0.75 | 0.5649 | 0.0086 |
| 155 | 85.36 | 11.60 | 17.83 | 0.9966 | 0.60 | 0.5457 | 0.0073 |
| 200 | 86.34 | 39.24 | 37.88 | 0.9982 | 0.43 | 0,5074 | 0,0056 |
| 65 | 20 | 92.98 | 23.62 | 11.27 | 0.9456 | 17.83 | 5.3701 | 0.1096 |
| 65 | 85.84 | 25.77 | 17.15 | 0.9922 | 2.07 | 1.2505 | 0.0232 |
| 110 | 84.25 | 14.96 | 15.33 | 0.9911 | 2.03 | 1.2900 | 0.0177 |
| 155 | 79.18 | 4.08 | 8.66 | 0.9976 | 0.91 | 0.5877 | 0.0076 |
| 200 | 84.63 | 16.43 | 22.88 | 0.9964 | 0.52 | 0.4686 | 0.0066 |
| 70 | 20 | 94.68 | 45.25 | 15.44 | 0.9304 | 18.16 | 6.0664 | 0.1379 |
| 65 | 91.04 | 14.91 | 10.65 | 0.9655 | 8.43 | 3.7035 | 0.0661 |
| 110 | 86.18 | 118.27 | 37.24 | 0.9843 | 3.79 | 2.0404 | 0.0296 |
| 155 | 83.47 | 13.36 | 13.42 | 0.9963 | 1.28 | 0.8194 | 0.0130 |
| 200 | 81.92 | 21.68 | 18.45 | 0.9981 | 0.84 | 0.5528 | 0.0080 |

Table 4S. Calculated model parameters and statistical parameters for Peleg’s model

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| T  [°C] | p  [mbar] | Adjustable coefficients | | *R*2 | AARD [%] | RMSE | *χ*2 |
|  |  | k1 | k2 |  |  |  |  |
| 50 | 20 | 0.2020 | -0.006821 | 0.6656 | 16.43 | 20.6470 | 0.3687 |
| 65 | 0.3440 | -0.008137 | 0.9967 | 1.43 | 0.9779 | 0.0124 |
| 110 | 0.5910 | -0.021667 | 0.9919 | 0.96 | 0.8563 | 0.0132 |
| 155 | 0.3096 | -0.000537 | 0.9950 | 0.79 | 0.8782 | 0.0113 |
| 200 | 0.2755 | 0.033735 | 0.9675 | 0.52 | 0.7758 | 0.0125 |
| 55 | 20 | 0.1901 | -0.006068 | 0.9966 | 2.70 | 1.2539 | 0.0224 |
| 65 | 0.2619 | 0.005383 | 0.9978 | 0.78 | 0.5599 | 0.0067 |
| 110 | 0.2600 | 0.012412 | 0.9821 | 1.49 | 1.2773 | 0.0129 |
| 155 | 0.4499 | 0.034336 | 0.9906 | 0.24 | 0.2972 | 0.0063 |
| 200 | 2.1998 | -0.054133 | 0.9442 | 0.57 | 0.7902 | 0.0094 |
| 60 | 20 | 0.1467 | -0.002025 | 0.9972 | 2.65 | 1.1134 | 0.0206 |
| 20 | 0.1972 | -0.009380 | 0.9982 | 1.34 | 0.7940 | 0.0173 |
| 20 | 0.1646 | -0.006348 | 0.9970 | 2.28 | 1.1142 | 0.0242 |
| 65 | 0.1806 | 0.000450 | 0.9988 | 0.85 | 0.5758 | 0.0093 |
| 110 | 0.1575 | 0.009105 | 0.9912 | 1.24 | 1.1266 | 0.0168 |
| 155 | 0.3196 | 0.006547 | 0.9967 | 0.58 | 0.5406 | 0.0071 |
| 200 | 0.4935 | 0.002330 | 0.9972 | 0.42 | 0.4545 | 0.0050 |
| 65 | 20 | 0.1119 | -0.000407 | 0.9965 | 4.30 | 1.3677 | 0.0274 |
| 65 | 0.1482 | 0.004547 | 0.9953 | 1.55 | 0.9761 | 0.0177 |
| 110 | 0.1913 | 0.005128 | 0.9925 | 1.61 | 1.1811 | 0.0160 |
| 155 | 0.1392 | 0.011333 | 0.9703 | 2.57 | 2.0455 | 0.0262 |
| 200 | 0.3258 | 0.010335 | 0.9978 | 0.42 | 0.3656 | 0.0051 |
| 70 | 20 | 0.1261 | -0.003570 | 0.9964 | 3.86 | 1.3865 | 0.0308 |
| 65 | 0.1457 | -0.000402 | 0.9984 | 1.60 | 0.8027 | 0.0141 |
| 110 | 0.1679 | 0.003174 | 0.9958 | 1.51 | 1.0589 | 0.0151 |
| 155 | 0.1440 | 0.007439 | 0.9940 | 1.42 | 1.0482 | 0.0164 |
| 200 | 0.1457 | 0.009295 | 0.9910 | 1.58 | 1.2123 | 0.0173 |

Table 5S. Calculated model parameters and statistical parameters for Logarithmic model

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| T  [°C] | p  [mbar] | Adjustable coefficients | | | *R*2 | AARD [%] | RMSE | *χ*2 |
|  |  | a | k | b |  |  |  |  |
| 50 | 20 | 71.08 | 0.1562 | 18.3132 | 0.8647 | 18.72 | 7.9405 | 0.1444 |
| 65 | -87.88 | -0.0380 | 175.2104 | 0.9990 | 0.78 | 0.5288 | 0.0068 |
| 110 | -38.27 | -0.0558 | 125.4604 | 0.9988 | 0.35 | 0.3241 | 0.0051 |
| 155 | -104.77 | -0.0257 | 188.1512 | 0.9978 | 0.75 | 0.5754 | 0.0075 |
| 200 | -134.44 | -0.0097 | 216.0966 | 0.9822 | 0.67 | 0.5749 | 0.0094 |
| 55 | 20 | 89.97 | 0.1248 | 1.6709 | 0.9281 | 14.12 | 5.7218 | 0.1040 |
| 65 | -327.34 | -0.0084 | 410.1009 | 0.9934 | 1.22 | 0.9744 | 0.0119 |
| 110 | -243.22 | -0.0075 | 322.8373 | 0.9945 | 0.89 | 0.7103 | 0.0072 |
| 155 | -76.04 | -0.0159 | 159.9115 | 0.9921 | 0.30 | 0.2728 | 0.0059 |
| 200 | -95.44 | -0.0079 | 182.3331 | 0.9914 | 0.30 | 0.3109 | 0.0037 |
| 60 | 20 | 54.30 | 0.2574 | 30.5029 | 0.8091 | 24.21 | 9.2307 | 0.1742 |
| 20 | -52.24 | -0.1019 | 138.6473 | 0.9991 | 1.00 | 0.5729 | 0.0127 |
| 20 | -77.57 | -0.0810 | 163.6971 | 0.9975 | 2.06 | 1.0089 | 0.0224 |
| 65 | -280.05 | -0.0175 | 364.1609 | 0.9979 | 1.06 | 0.7622 | 0.0125 |
| 110 | -401.63 | -0.0085 | 481.3118 | 0.9917 | 1.59 | 1.0888 | 0.0165 |
| 155 | -244.90 | -0.0095 | 328.6115 | 0.9902 | 0.99 | 0.9262 | 0.0123 |
| 200 | -218.15 | -0.0082 | 303.1148 | 0.9948 | 0.69 | 0.6201 | 0.0069 |
| 65 | 20 | 100.97 | 0.1530 | -10.2785 | 0.9595 | 15.07 | 4.6346 | 0.0946 |
| 65 | -309.40 | -0.0154 | 391.4782 | 0.9919 | 1.60 | 1.2772 | 0.0237 |
| 110 | -273.26 | -0.0126 | 354.0613 | 0.9978 | 0.87 | 0.6363 | 0.0087 |
| 155 | -331.81 | -0.0087 | 408.1544 | 0.9939 | 1.38 | 0.9302 | 0.0121 |
| 200 | -202.69 | -0.0101 | 286.0865 | 0.9876 | 1.04 | 0.8741 | 0.0123 |
| 70 | 20 | 101.48 | 0.1616 | -8.7688 | 0.9426 | 16.29 | 5.5086 | 0.1252 |
| 65 | -273.92 | -0.0228 | 358.0488 | 0.9981 | 1.82 | 0.8614 | 0.0154 |
| 110 | -276.40 | -0.0154 | 357.6031 | 0.9979 | 1.24 | 0.7506 | 0.0109 |
| 155 | -393.33 | -0.0101 | 473.2542 | 0.9909 | 1.81 | 1.2904 | 0.0205 |
| 200 | -450.33 | -0.0077 | 529.1043 | 0.9904 | 1.78 | 1.2406 | 0.0180 |

Table 6S. Calculated model parameters and statistical parameters for Two-term model

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| T  [°C] | p  [mbar] | Adjustable coefficients | | | | *R*2 | AARD [%] | RMSE | *χ*2 |
|  |  | a | k1 | b | k2 |  |  |  |  |
| 50 | 20 | 48.08 | 0.1312 | 48.08 | 0.1311 | 0.9277 | 13.33 | 5.8062 | 0.1075 |
| 65 | 46.49 | 0.0689 | 46.49 | 0.0689 | 0.9641 | 5.33 | 3.2037 | 0.0416 |
| 110 | 44.82 | 0.0398 | 44.82 | 0.0398 | 0.9794 | 1.62 | 1.3607 | 0.0216 |
| 155 | 43.21 | 0.0497 | 43.21 | 0.0497 | 0.9803 | 2.38 | 1.7355 | 0.0228 |
| 200 | 68.97 | 0.0364 | 13.78 | -0.0404 | 0.9955 | 0.28 | 0.2879 | 0.0048 |
| 55 | 20 | 47.57 | 0.1328 | 47.57 | 0.1328 | 0.9369 | 12.42 | 5.3606 | 0.0993 |
| 65 | 42.71 | 0.0467 | 42.71 | 0.0467 | 0.9970 | 0.92 | 0.6543 | 0.0081 |
| 110 | 40.70 | 0.0308 | 40.70 | 0.0308 | 0.9984 | 0.49 | 0.3813 | 0.0039 |
| 155 | 60.36 | 0.0018 | 24.04 | 0.0632 | 0.9981 | 0.14 | 0.1320 | 0.0029 |
| 200 | 74.54 | 0.0043 | 12.97 | 0.0551 | 0.9974 | 0.17 | 0.1714 | 0.0021 |
| 60 | 20 | 46.43 | 0.1455 | 46.43 | 0.1455 | 0.9527 | 11.18 | 4.5943 | 0.0884 |
| 20 | 46.91 | 0.1311 | 46.91 | 0.1311 | 0.9421 | 8.58 | 4.5152 | 0.1026 |
| 20 | 46.96 | 0.1490 | 46.96 | 0.1490 | 0.9402 | 10.58 | 4.9472 | 0.1124 |
| 65 | 44.52 | 0.0937 | 44.52 | 0.0937 | 0.9840 | 3.75 | 2.1043 | 0.0351 |
| 110 | 41.22 | 0.0605 | 41.19 | 0.0605 | 0.9978 | 0.75 | 0.5649 | 0.0087 |
| 155 | 11.59 | 0.0775 | 73.97 | 0.0316 | 0.9967 | 0.62 | 0.5401 | 0.0073 |
| 200 | 43.17 | 0.0273 | 43.17 | 0.0273 | 0.9982 | 0.45 | 0.3641 | 0.0041 |
| 65 | 20 | 46.49 | 0.1861 | 46.49 | 0.1860 | 0.9456 | 17.83 | 5.3701 | 0.1119 |
| 65 | 42.92 | 0.0876 | 42.92 | 0.0876 | 0.9922 | 2.07 | 1.2505 | 0.0236 |
| 110 | 42.12 | 0.0636 | 42.12 | 0.0636 | 0.9912 | 2.03 | 1.2900 | 0.0179 |
| 155 | 39.59 | 0.0545 | 39.59 | 0.0545 | 0.9975 | 0.91 | 0.5877 | 0.0077 |
| 200 | 4.21 | 0.2556 | 81.34 | 0.0276 | 0.9981 | 0.38 | 0.3459 | 0.0049 |
| 70 | 20 | 47.34 | 0.1896 | 47.34 | 0.1898 | 0.9304 | 18.16 | 6.0664 | 0.1411 |
| 65 | 45.52 | 0.1315 | 45.52 | 0.1315 | 0.9655 | 8.43 | 3.7035 | 0.0673 |
| 110 | 43.09 | 0.0853 | 43.09 | 0.0853 | 0.9843 | 3.79 | 2.0404 | 0.0300 |
| 155 | 41.74 | 0.0741 | 41.74 | 0.0741 | 0.9963 | 1.28 | 0.8194 | 0.0132 |
| 200 | 40.96 | 0.0637 | 40.96 | 0.0637 | 0.9981 | 0.84 | 0.5528 | 0.0081 |