Optimization of the direct synthesis of dimethyl ether from CO₂ rich synthesis gas: Closing the loop between experimental investigations and model-based reactor design

Nirvana Delgado Otalvaro¹,², Markus Kaiser¹, Karla Herrera Delgado³, Stefan Wild³, Jörg Sauer³, and Hannsjörg Freund¹

¹Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Lehrstuhl für Chemische Reaktionstechnik, IZNF, Cauerstr. 3, D-91058 Erlangen, Germany.
²Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany.

Electronic Supplementary Information

Section 2.1 Experimental setup

The experimental setup depicted in Figure 1 was used to conduct kinetic measurements and the experimental validation of model-based optimization results.

Figure 1: Flow diagram of the experimental setup.
The gas supply is regulated via mass flow controller (MFC, Bronkhorst High Tech, FIRC 1, 2, 3, 4 and 5) by using proportional-integral-derivative (PID) control.

The tube reactor consists of a vertical cylinder made of the stainless steel 1.4571. The reactor is designed for temperatures up to 350 °C and a maximal pressure of 100 bar. The thermocouple used for the temperature measurement over the reactor length is of the type K, NiCr-Ni. To ensure isothermal operating conditions the catalyst bed was diluted with SiC. Two exemplary temperature profiles measured with thermocouples along the axial direction during the experiments are shown in Figure 2 and 3.

The temperature profiles were measured with a scale division of 0.5 cm for the catalyst bed position. Temperature values were recorded under steady state conditions.
The Gas Chromatograph (GC) G1530A from Agilent Technologies is equipped with a thermal conductivity detector (TCD), a flame ionization detector (FID), an automatic loop filling manager system from Teuner Analysentechnik GmbH (LFM 205) and two capillary columns RT-Msieve 5A and RT-U-BOND from Restek Corporation.

For the kinetic studies, mixtures of a commercially available CuO/ZnO/α-Al₂O₃ (CZA) catalyst provided by an industrial partner, γ-Al₂O₃ (ALOX, Alfa Aesar) and silicon carbide (SiC, Hausen Mineraľengroßhandel GmbH) were used.

The reactant gases carbon monoxide (CO, 99.97 %), argon (Ar, 99.9999 %), nitrogen (N₂, 99.9999 %), Hydrogen (H₂, 9.9999 %) and mixture carbon dioxide and nitrogen (CO₂/N₂, 50:50 ± 1.0 vol. %) were provided by Air Liquid Germany GmbH.

**Section 3.1 Reaction kinetic measurements**

The measured kinetic data used for the parameter estimation of the lumped kinetic model are provided in Table 1.

The reader is advised:

- The feed gas consisted of Hydrogen, Carbon Monoxide, Carbon Dioxide and inert gas (Argon and Nitrogen). Only the concentration of the reactive components is reported here.
- Each operating point was measured under steady state conditions for approx. 90 Minutes. Possible deviations and fluctuations of the reported temperature and inlet volume flow are here neglected.
## Table 1: Measured kinetic data

| Exp. ID | Temp. °C | Inlet Vol. g | Mass CZA-Cat. g | Mass ALOX-Cat. g | Cat. Bed Length m | H₂ in Feed Vol. % | CO in Feed Vol. % | CO₂ in Feed Vol. % | H₂ in Product Vol. % | CO in Product Vol. % | CO₂ in Product Vol. % | DME in Product Vol. % |
|---------|----------|--------------|-----------------|------------------|------------------|-------------------|-----------------|-------------------|---------------------|-------------------|-------------------|---------------------|
| 1       | 220      | 0.7          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 47.95%          | 16.06%           | 2.883%              | 46.757%           | 15.264%           | 2.8206%             |
| 2       | 220      | 0.6          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 47.99%          | 16.11%           | 2.880%              | 46.759%           | 15.277%           | 2.8282%             |
| 3       | 220      | 0.5          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 47.97%          | 16.09%           | 2.880%              | 46.633%           | 15.091%           | 2.8310%             |
| 4       | 220      | 0.4          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 47.69%          | 15.75%           | 2.847%              | 46.679%           | 14.987%           | 2.9265%             |
| 5       | 220      | 0.3          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 48.11%          | 15.91%           | 2.853%              | 46.602%           | 14.820%           | 3.0040%             |
| 6       | 220      | 0.2          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 48.42%          | 15.07%           | 2.814%              | 46.086%           | 13.852%           | 3.3271%             |
| 7       | 230      | 0.7          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 47.95%          | 16.06%           | 2.883%              | 46.403%           | 14.776%           | 2.9888%             |
| 8       | 230      | 0.6          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 47.99%          | 16.11%           | 2.883%              | 46.481%           | 14.770%           | 2.9967%             |
| 9       | 230      | 0.5          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 47.97%          | 16.09%           | 2.881%              | 46.251%           | 14.579%           | 3.0496%             |
| 10      | 230      | 0.4          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 47.69%          | 15.75%           | 2.847%              | 46.241%           | 14.313%           | 3.2145%             |
| 11      | 230      | 0.3          | 1.000 g         | 1.001 g          | 5.000 g          | 0.054 g           | 48.11%          | 15.91%           | 2.853%              | 45.935%           | 13.905%           | 3.3430%             |
| 12 | 230 | 0.2 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 48.42 00 | 16.07 24 | 2.814 8 | 45.055 8 | 12.255 2 | 3.9595 1.3078 |
| 13 | 240 | 0.7 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 47.95 21 | 16.06 18 | 2.883 5 | 45.837 3 | 13.990 8 | 3.2840 0.6447 |
| 14 | 240 | 0.6 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 47.99 64 | 16.11 22 | 2.883 0 | 45.857 1 | 13.984 4 | 3.2881 0.6505 |
| 15 | 240 | 0.5 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 47.97 60 | 16.09 05 | 2.881 1 | 45.449 0 | 13.649 0 | 3.3512 0.7593 |
| 16 | 240 | 0.4 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 47.69 62 | 15.75 91 | 2.847 6 | 45.628 3 | 13.241 2 | 3.6648 1.0165 |
| 17 | 240 | 0.3 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 48.11 76 | 15.91 25 | 2.853 4 | 45.107 8 | 12.563 2 | 3.8949 1.2982 |
| 18 | 240 | 0.2 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 48.42 00 | 16.07 24 | 2.814 8 | 43.990 3 | 10.161 2 | 4.8538 2.2916 |
| 19 | 250 | 0.7 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 47.95 21 | 16.06 18 | 2.883 5 | 45.187 0 | 12.912 6 | 3.7566 1.1476 |
| 20 | 250 | 0.6 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 47.99 64 | 15.91 22 | 2.883 0 | 44.848 5 | 12.697 2 | 3.7438 1.1509 |
| 21 | 250 | 0.5 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 47.97 60 | 16.09 05 | 2.881 1 | 44.656 7 | 12.367 3 | 3.8704 1.3352 |
| 22 | 250 | 0.4 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 47.69 62 | 15.75 91 | 2.847 6 | 44.708 9 | 11.723 2 | 4.2624 1.7025 |
| 23 | 250 | 0.3 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 48.11 76 | 15.91 25 | 2.853 4 | 44.082 4 | 10.750 4 | 4.6558 2.1266 |
| 24 | 250 | 0.2 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 48.42 00 | 16.07 24 | 2.814 8 | 42.839 3 | 7.8665 3 | 5.8356 3.3782 |
| 25 | 260 | 0.7 | 1.000 2 | 1.001 7 | 5.000 0 | 0.054 5 | 47.95 21 | 16.06 18 | 2.883 5 | 44.578 7 | 11.665 9 | 4.2707 1.7367 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 26 | 260 | 0.6 | 1.000 | 2 | 1.001 | 7 | 5.000 | 0 | 0.054 | 5 | 47.99 | 64 | 16.11 | 22 | 2.883 |
| 27 | 260 | 0.5 | 1.000 | 2 | 1.001 | 7 | 5.000 | 0 | 0.054 | 5 | 47.97 | 60 | 16.09 | 05 | 2.881 |
| 28 | 260 | 0.4 | 1.000 | 2 | 1.001 | 7 | 5.000 | 0 | 0.054 | 5 | 47.69 | 62 | 15.75 | 91 | 2.847 |
| 29 | 260 | 0.3 | 1.000 | 2 | 1.001 | 7 | 5.000 | 0 | 0.054 | 5 | 48.11 | 76 | 15.91 | 25 | 2.853 |
| 30 | 260 | 0.2 | 1.000 | 2 | 1.001 | 7 | 5.000 | 0 | 0.054 | 5 | 48.42 | 00 | 16.07 | 24 | 2.814 |
| 31 | 220 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.23 | 71 | 8.333 | 1 | 2.902 |
| 32 | 220 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.15 | 34 | 8.177 | 9 | 2.809 |
| 33 | 220 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.28 | 31 | 8.287 | 6 | 2.854 |
| 34 | 220 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.28 | 31 | 8.287 | 6 | 2.854 |
| 35 | 220 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.11 | 09 | 8.353 | 2 | 2.945 |
| 36 | 220 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.25 | 12 | 8.373 | 7 | 2.880 |
| 37 | 230 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.23 | 71 | 8.333 | 1 | 2.902 |
| 38 | 230 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.15 | 34 | 8.177 | 9 | 2.809 |
| 39 | 230 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.28 | 31 | 8.287 | 6 | 2.854 |
| 40 | 230 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.28 | 8.287 | 2.854 | 28.750 | 7.2033 | 3.0519 | 0.3946 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 41 | 230 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.11 | 09 | 8.353 | 2 | 2.945 | 1 |
| 42 | 230 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.25 | 12 | 8.373 | 7 | 2.880 | 4 |
| 43 | 240 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.23 | 71 | 8.333 | 1 | 2.902 | 4 |
| 44 | 240 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.15 | 34 | 8.177 | 9 | 2.809 | 6 |
| 45 | 240 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.28 | 31 | 8.287 | 6 | 2.854 | 7 |
| 46 | 240 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.28 | 31 | 8.287 | 6 | 2.854 | 7 |
| 47 | 240 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.11 | 09 | 8.353 | 2 | 2.945 | 1 |
| 48 | 240 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.25 | 12 | 8.373 | 7 | 2.880 | 4 |
| 49 | 250 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.23 | 71 | 8.333 | 1 | 2.902 | 4 |
| 50 | 250 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.15 | 34 | 8.177 | 9 | 2.809 | 6 |
| 51 | 250 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.28 | 31 | 8.287 | 6 | 2.854 | 7 |
| 52 | 250 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.28 | 31 | 8.287 | 6 | 2.854 | 7 |
| 53 | 250 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.11 | 09 | 8.353 | 2 | 2.945 | 1 |
| 54 | 250 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 30.25 | 12 | 8.373 | 7 | 2.880 | 4 |
|   |   | 0.7 | 1.000 | 1.001 | 10.00 | 0.080 | 30.23 | 8.333 | 2.902 | 28.274 | 6.7380 | 3.2400 | 0.6188 |
|---|---|-----|-------|-------|-------|-------|-------|-------|-------|---------|---------|---------|--------|
| 55| 260| 0.6  | 1.000 | 1.001 | 10.00 | 0.080 | 30.15 | 8.177 | 2.809 | 27.837 | 6.0005 | 3.4991 | 0.9141 |
| 56| 260| 0.8  | 1.000 | 1.001 | 10.00 | 0.080 | 30.28 | 8.287 | 2.854 | 27.614 | 5.7184 | 3.5971 | 1.0343 |
| 57| 260| 0.4  | 1.000 | 1.001 | 10.00 | 0.080 | 30.28 | 8.287 | 2.854 | 27.246 | 5.2907 | 3.7708 | 1.2109 |
| 58| 260| 0.3  | 1.000 | 1.001 | 10.00 | 0.080 | 30.11 | 8.353 | 2.945 | 26.669 | 4.5852 | 3.9625 | 1.4868 |
| 59| 260| 0.2  | 1.000 | 1.001 | 10.00 | 0.080 | 30.22 | 8.373 | 2.880 | 26.018 | 3.6080 | 4.3567 | 1.9090 |
| 60| 220| 0.7  | 1.000 | 1.001 | 10.00 | 0.080 | 20.37 | 4.118 | 2.859 | 19.808 | 3.9426 | 2.7458 | 0.0657 |
| 61| 220| 0.6  | 1.000 | 1.001 | 10.00 | 0.080 | 20.37 | 4.118 | 2.859 | 19.671 | 3.9061 | 2.7453 | 0.0744 |
| 62| 220| 0.5  | 1.000 | 1.001 | 10.00 | 0.080 | 20.17 | 4.045 | 2.883 | 19.519 | 3.8318 | 2.7799 | 0.0923 |
| 63| 220| 0.4  | 1.000 | 1.001 | 10.00 | 0.080 | 20.17 | 4.045 | 2.883 | 19.442 | 3.7183 | 2.8087 | 0.1229 |
| 64| 220| 0.3  | 1.000 | 1.001 | 10.00 | 0.080 | 20.22 | 4.008 | 2.849 | 19.477 | 3.5695 | 2.8672 | 0.1724 |
| 65| 220| 0.2  | 1.000 | 1.001 | 10.00 | 0.080 | 20.33 | 4.050 | 2.862 | 19.497 | 3.2875 | 2.9309 | 0.2794 |
| 66| 230| 0.7  | 1.000 | 1.001 | 10.00 | 0.080 | 20.37 | 4.118 | 2.859 | 19.637 | 3.8179 | 2.7495 | 0.1114 |
| 67| 230| 0.6  | 1.000 | 1.001 | 10.00 | 0.080 | 20.37 | 4.118 | 2.859 | 19.489 | 3.7667 | 2.7689 | 0.1285 |
| 68| 230| 0.5  | 1.000 | 1.001 | 10.00 | 0.080 | 20.17 | 4.045 | 2.883 | 19.322 | 3.6605 | 2.8114 | 0.1559 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 70 | 230 | 0.4 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.1765 | 4.0458 | 2.8830 | 19.2407 | 3.5196 | 2.8461 | 0.2020 |
| 71 | 230 | 0.3 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.2229 | 4.0085 | 2.8496 | 19.3213 | 3.3273 | 2.9407 | 0.2775 |
| 72 | 230 | 0.2 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.3301 | 4.0507 | 2.8626 | 19.1740 | 2.9323 | 3.0258 | 0.4218 |
| 73 | 240 | 0.7 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.3739 | 4.1180 | 2.8595 | 19.4997 | 3.6736 | 2.8073 | 0.1765 |
| 74 | 240 | 0.6 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.3739 | 4.1180 | 2.8595 | 19.2797 | 3.5911 | 2.8033 | 0.2030 |
| 75 | 240 | 0.5 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.1765 | 4.0458 | 2.8830 | 19.1832 | 3.4863 | 2.8768 | 0.2415 |
| 76 | 240 | 0.4 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.1765 | 4.0458 | 2.8830 | 19.0363 | 3.3077 | 2.9388 | 0.2992 |
| 77 | 240 | 0.3 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.2229 | 4.0085 | 2.8496 | 19.1106 | 3.0527 | 3.0197 | 0.3999 |
| 78 | 240 | 0.2 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.3301 | 4.0507 | 2.8626 | 18.7834 | 2.5695 | 3.1438 | 0.5700 |
| 79 | 250 | 0.7 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.3739 | 4.1180 | 2.8595 | 19.3207 | 3.5212 | 2.8476 | 0.2505 |
| 80 | 250 | 0.6 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.3739 | 4.1180 | 2.8595 | 19.1090 | 3.4051 | 2.8903 | 0.2851 |
| 81 | 250 | 0.5 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.1765 | 4.0458 | 2.8830 | 19.0055 | 3.2768 | 2.9561 | 0.3314 |
| 82 | 250 | 0.4 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.1765 | 4.0458 | 2.8830 | 18.7817 | 3.0787 | 2.9893 | 0.4006 |
| 83 | 250 | 0.3 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 20.2229 | 4.0085 | 2.8496 | 18.8603 | 2.7960 | 3.0871 | 0.5085 |
| 84 | 250 | 0.2 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 20.33 01 | 4.050 7 | 2.862 6 | 18.598 3 | 2.3130 | 3.1967 | 0.6835 |
| 85 | 260 | 0.7 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 20.37 39 | 4.118 00 | 2.859 5 | 19.149 0 | 3.3891 | 2.8903 | 0.3131 |
| 86 | 260 | 0.6 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 20.37 39 | 4.118 00 | 2.859 5 | 19.002 9 | 3.2503 | 2.9465 | 0.3527 |
| 87 | 260 | 0.5 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 20.17 65 | 4.045 8 | 2.883 0 | 18.816 7 | 3.1226 | 2.9831 | 0.4013 |
| 88 | 260 | 0.4 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 20.17 65 | 4.045 8 | 2.883 0 | 18.576 2 | 2.9056 | 3.0461 | 0.4704 |
| 89 | 260 | 0.3 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 20.22 29 | 4.008 5 | 2.849 6 | 18.650 2 | 2.6586 | 3.1209 | 0.5726 |
| 90 | 260 | 0.2 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 20.33 01 | 4.050 7 | 2.862 6 | 18.440 7 | 2.2483 | 3.2382 | 0.7175 |
| 91 | 220 | 0.7 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 41.28 34 | 15.81 43 | 0.909 3 | 40.898 2 | 15.465 2 | 0.9273 | 0.1296 |
| 92 | 220 | 0.6 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 41.28 34 | 15.81 43 | 0.909 3 | 41.083 0 | 15.536 4 | 0.9760 | 0.1850 |
| 93 | 220 | 0.5 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 41.67 09 | 15.98 54 | 0.911 3 | 41.039 9 | 15.470 7 | 1.0148 | 0.2462 |
| 94 | 220 | 0.4 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 41.67 09 | 15.98 54 | 0.911 3 | 40.865 9 | 15.262 5 | 1.0735 | 0.3395 |
| 95 | 220 | 0.3 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 41.84 97 | 16.06 62 | 0.894 7 | 40.619 9 | 14.943 1 | 1.1611 | 0.4713 |
| 96 | 220 | 0.2 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 42.32 76 | 16.13 62 | 0.819 2 | 39.733 9 | 14.157 8 | 1.4173 | 0.8071 |
| 97 | 230 | 0.7 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 41.28 34 | 15.81 43 | 0.909 3 | 40.771 4 | 15.242 9 | 1.0121 | 0.2388 |
| 98 | 230 | 0.6 | 1.000 2 | 1.001 7 | 10.00 00 | 0.080 00 | 41.28 15 | 15.81 43 | 0.909 3 | 40.911 | 15.231 | 1.1026 | 0.3269 |
|   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 99 | 230 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.67 | 09 | 15.98 | 54 | 0.911 | 3 | 40.755 | 2 | 15.027 | 0 | 1.1637 | 0.4242 |
| 100 | 230 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.67 | 09 | 15.98 | 54 | 0.911 | 3 | 40.429 | 4 | 14.714 | 8 | 1.2708 | 0.5729 |
| 101 | 230 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.84 | 97 | 16.06 | 62 | 0.894 | 7 | 40.010 | 3 | 14.188 | 1 | 1.4312 | 0.7828 |
| 102 | 230 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 42.32 | 76 | 16.13 | 62 | 0.819 | 2 | 38.944 | 2 | 12.969 | 8 | 1.8464 | 1.3010 |
| 103 | 240 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.28 | 34 | 15.81 | 43 | 0.909 | 3 | 40.425 | 9 | 14.807 | 2 | 1.1584 | 0.4117 |
| 104 | 240 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.28 | 34 | 15.81 | 43 | 0.909 | 3 | 40.610 | 5 | 14.781 | 5 | 1.2878 | 0.5467 |
| 105 | 240 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.67 | 09 | 15.98 | 54 | 0.911 | 3 | 40.208 | 6 | 14.350 | 8 | 1.4003 | 0.6977 |
| 106 | 240 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.67 | 09 | 15.98 | 54 | 0.911 | 3 | 39.921 | 6 | 13.934 | 2 | 1.5756 | 0.9266 |
| 107 | 240 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.84 | 97 | 16.06 | 62 | 0.894 | 7 | 39.133 | 9 | 13.048 | 3 | 1.8323 | 1.2556 |
| 108 | 240 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 42.32 | 76 | 16.13 | 62 | 0.819 | 2 | 37.873 | 6 | 11.374 | 2 | 2.4964 | 2.0382 |
| 109 | 250 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.28 | 34 | 15.81 | 43 | 0.909 | 3 | 40.006 | 1 | 14.199 | 0 | 1.3890 | 0.6812 |
| 110 | 250 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.28 | 34 | 15.81 | 43 | 0.909 | 3 | 40.055 | 8 | 14.011 | 4 | 1.5600 | 0.8783 |
| 111 | 250 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.67 | 09 | 15.98 | 54 | 0.911 | 3 | 39.641 | 1 | 13.467 | 7 | 1.7418 | 1.1102 |
| 112 | 250 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.67 | 09 | 15.98 | 54 | 0.911 | 3 | 39.006 | 9 | 12.721 | 7 | 2.0205 | 1.4307 |
| Page | 250 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.84 | 97 | 16.06 | 62 | 0.894 | 7 | 38.086 | 7 | 11.517 | 1 | 2.4156 | 1.9394 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 114 | 250 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 42.32 | 76 | 16.13 | 62 | 0.819 | 2 | 36.338 | 2 | 9.1713 | 3 | 3.2742 | 2.9509 |
| 115 | 260 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.28 | 34 | 15.81 | 43 | 0.909 | 3 | 39.421 | 3 | 13.333 | 8 | 1.7268 | 1.0742 |
| 116 | 260 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.28 | 34 | 15.81 | 43 | 0.909 | 3 | 39.291 | 3 | 12.929 | 5 | 1.9652 | 1.3370 |
| 117 | 260 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.67 | 09 | 15.98 | 54 | 0.911 | 3 | 38.630 | 2 | 12.173 | 4 | 2.2193 | 1.6576 |
| 118 | 260 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.67 | 09 | 15.98 | 54 | 0.911 | 3 | 37.968 | 8 | 11.206 | 4 | 2.5730 | 2.0891 |
| 119 | 260 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 41.84 | 97 | 16.06 | 62 | 0.894 | 7 | 36.699 | 3 | 9.6157 | 4 | 3.1148 | 2.7614 |
| 120 | 260 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 42.32 | 76 | 16.13 | 62 | 0.819 | 2 | 35.047 | 0 | 7.0272 | 0 | 4.1437 | 3.9770 |
| 121 | 220 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.95 | 62 | 8.481 | 4 | 0.885 | 9 | 23.217 | 0 | 8.0966 | 0 | 0.9005 | 0.1232 |
| 122 | 220 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.89 | 21 | 8.474 | 5 | 0.878 | 5 | 23.314 | 4 | 8.1380 | 0 | 0.9153 | 0.1322 |
| 123 | 220 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.81 | 56 | 8.555 | 2 | 0.852 | 3 | 23.149 | 0 | 8.0504 | 0 | 0.9519 | 0.1787 |
| 124 | 220 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.81 | 56 | 8.555 | 2 | 0.852 | 3 | 23.608 | 5 | 7.9027 | 9 | 0.9906 | 0.2340 |
| 125 | 220 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.85 | 91 | 8.588 | 6 | 0.825 | 9 | 22.868 | 1 | 7.6531 | 0 | 1.0384 | 0.3368 |
| 126 | 220 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 24.02 | 15 | 8.569 | 7 | 0.764 | 0 | 22.664 | 7 | 7.2701 | 0 | 1.1547 | 0.5221 |
| 127 | 230 | 0.7 | 1.000 | 1 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.95 | 84 | 8.481 | 8 | 0.885 | 0 | 23.047 | 7 | 7.9275 | 9 | 0.9889 | 0.1977 |
| Row | 2 | 7 | 00 | 62 | 4 | 9 | 3 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 |
|-----|---|---|----|----|---|---|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 128 | 230 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.89 | 8.474 | 5 | 0.878 | 5 | 23.128 | 2 | 7.9371 | 1.0048 | 0.2192 |
| 129 | 230 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.81 | 8.555 | 2 | 0.852 | 3 | 22.934 | 0 | 7.7698 | 1.0501 | 0.2845 |
| 130 | 230 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.81 | 8.555 | 2 | 0.852 | 3 | 23.436 | 8 | 7.5664 | 1.1161 | 0.3714 |
| 131 | 230 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.85 | 8.588 | 6 | 0.825 | 9 | 22.540 | 9 | 7.2095 | 1.1883 | 0.5121 |
| 132 | 230 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 24.02 | 8.569 | 7 | 0.764 | 0 | 22.032 | 9 | 6.5939 | 1.3721 | 0.7841 |
| 133 | 240 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.95 | 8.481 | 4 | 0.885 | 9 | 22.829 | 7 | 7.6373 | 1.0866 | 0.3090 |
| 134 | 240 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.89 | 8.474 | 5 | 0.878 | 5 | 22.859 | 7 | 7.6164 | 1.1075 | 0.3449 |
| 135 | 240 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.81 | 8.555 | 2 | 0.852 | 3 | 22.663 | 5 | 7.4010 | 1.1844 | 0.4359 |
| 136 | 240 | 0.4 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.81 | 8.555 | 2 | 0.852 | 3 | 22.517 | 5 | 7.1155 | 1.2804 | 0.5525 |
| 137 | 240 | 0.3 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.85 | 8.588 | 6 | 0.825 | 9 | 22.012 | 6 | 6.5926 | 1.3919 | 0.7542 |
| 138 | 240 | 0.2 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 24.02 | 8.569 | 7 | 0.764 | 0 | 21.281 | 0 | 5.7053 | 1.6789 | 1.1271 |
| 139 | 250 | 0.7 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.95 | 8.481 | 4 | 0.885 | 9 | 22.449 | 2 | 7.2782 | 1.1941 | 0.4486 |
| 140 | 250 | 0.6 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.89 | 8.474 | 5 | 0.878 | 5 | 22.527 | 8 | 7.2016 | 1.2531 | 0.5126 |
| 141 | 250 | 0.5 | 1.000 | 2 | 1.001 | 7 | 10.00 | 00 | 0.080 | 0 | 23.81 | 8.555 | 2 | 0.852 | 3 | 22.186 | 6 | 6.8944 | 1.3496 | 0.6280 |
| 142 | 250  | 0.4 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 23.815 | 8.555 | 2 | 0.852 | 3 | 21.990 | 5 | 6.5179 | 1.4779 | 0.7940 |
|------|------|----|--------|--------|--------|-------|---|--------|------|---|--------|---|--------|---|--------|------|------|
| 143 | 250  | 0.3 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 23.850 | 8.588 | 6 | 0.825 | 9 | 21.364 | 8 | 5.8472 | 1.6505 | 1.0493 |
| 144 | 250  | 0.2 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 24.020 | 8.569 | 7 | 0.764 | 0 | 20.391 | 8 | 4.7508 | 1.9806 | 1.4958 |
| 145 | 260  | 0.7 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 23.950 | 8.481 | 4 | 0.885 | 9 | 22.280 | 4 | 6.9234 | 1.3520 | 0.6173 |
| 146 | 260  | 0.6 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 23.890 | 8.474 | 5 | 0.878 | 5 | 22.044 | 7 | 6.7020 | 1.4120 | 0.7052 |
| 147 | 260  | 0.5 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 23.810 | 8.555 | 2 | 0.852 | 3 | 21.762 | 4 | 6.3559 | 1.5370 | 0.8444 |
| 148 | 260  | 0.4 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 23.810 | 8.555 | 2 | 0.852 | 3 | 21.432 | 2 | 5.8775 | 1.6871 | 1.0413 |
| 149 | 260  | 0.3 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 23.850 | 8.588 | 6 | 0.825 | 9 | 20.710 | 2 | 5.1354 | 1.8776 | 1.3149 |
| 150 | 260  | 0.2 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 24.020 | 8.569 | 7 | 0.764 | 0 | 19.765 | 7 | 4.0504 | 2.2075 | 1.7679 |
| 151 | 220  | 0.7 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 13.040 | 4.102 | 6 | 0.864 | 6 | 12.368 | 7 | 3.9014 | 0.8990 | 0.0984 |
| 152 | 220  | 0.6 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 13.040 | 4.102 | 6 | 0.864 | 6 | 12.292 | 4 | 3.8293 | 0.9214 | 0.1266 |
| 153 | 220  | 0.5 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 12.790 | 4.174 | 9 | 0.853 | 7 | 12.245 | 2 | 3.7663 | 0.9342 | 0.1627 |
| 154 | 220  | 0.4 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 12.790 | 4.174 | 9 | 0.853 | 7 | 12.452 | 8 | 3.7700 | 0.9477 | 0.1751 |
| 155 | 220  | 0.3 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 12.910 | 4.228 | 4 | 0.807 | 0 | 12.253 | 5 | 3.5891 | 0.9668 | 0.2487 |
| 156 | 220  | 0.2 | 1.000  | 1.001  | 10.000 | 0.080 | 0 | 13.090 | 4.264 | 7 | 0.757 | 0 | 11.927 | 5 | 3.3229 | 1.0013 | 0.3578 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 157 | 230 | 0.7 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 13.0499 | 4.1026 | 0.8646 | 12.2196 | 3.7518 | 0.9408 | 0.1499 |
| 158 | 230 | 0.6 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 13.0499 | 4.1026 | 0.8646 | 12.2068 | 3.6770 | 0.9636 | 0.1875 |
| 159 | 230 | 0.5 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 12.7918 | 4.1749 | 0.8537 | 12.1600 | 3.6261 | 0.9911 | 0.2225 |
| 160 | 230 | 0.4 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 12.7918 | 4.1749 | 0.8537 | 12.1578 | 3.5197 | 1.0093 | 0.2578 |
| 161 | 230 | 0.3 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 12.9164 | 4.2284 | 0.8070 | 11.9959 | 3.3062 | 1.0493 | 0.3463 |
| 162 | 230 | 0.2 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 13.0945 | 4.2642 | 0.7574 | 11.6456 | 2.9711 | 1.1019 | 0.4865 |
| 163 | 240 | 0.7 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 13.0499 | 4.1026 | 0.8646 | 12.0583 | 3.5966 | 0.9945 | 0.2151 |
| 164 | 240 | 0.6 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 13.0499 | 4.1026 | 0.8646 | 12.0163 | 3.5149 | 1.0288 | 0.2558 |
| 165 | 240 | 0.5 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 12.7918 | 4.1749 | 0.8537 | 11.9634 | 3.4135 | 1.0653 | 0.3061 |
| 166 | 240 | 0.4 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 12.7918 | 4.1749 | 0.8537 | 11.8705 | 3.2864 | 1.0971 | 0.3538 |
| 167 | 240 | 0.3 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 12.9164 | 4.2284 | 0.8070 | 11.7205 | 2.9828 | 1.1561 | 0.4609 |
| 168 | 240 | 0.2 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 13.0945 | 4.2642 | 0.7574 | 11.2967 | 2.5965 | 1.2235 | 0.6183 |
| 169 | 250 | 0.7 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 13.0499 | 4.1026 | 0.8646 | 11.8955 | 3.4241 | 1.0450 | 0.2816 |
| 170 | 250 | 0.6 | 1.0002 | 1.0017 | 10.0000 | 0.0800 | 13.0499 | 4.1026 | 0.8646 | 11.8371 | 3.3364 | 1.0909 | 0.3265 |
| Page | 171 | 172 | 173 | 174 | 175 | 176 | 177 | 178 | 179 | 180 | 181 | 182 | 183 | 184 | 185 |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 184  | 230 | 0.6 | 1.000| 0.000| 5.000| 0.035| 47.05| 51  | 15.40| 21  | 2.879| 5   | 44.841| 9   | 14.200| 1   |
| 183  | 220 | 0.5 | 1.000| 0.000| 5.000| 0.035| 48.98| 91  | 15.34| 84  | 2.851| 2   | 46.938| 7   | 15.025| 0   |
| 182  | 220 | 0.4 | 1.000| 0.000| 5.000| 0.035| 48.98| 91  | 16.06| 47  | 2.939| 0   | 43.977| 3   | 13.819| 7   |
| 181  | 220 | 0.6 | 1.000| 0.000| 5.000| 0.035| 47.05| 51  | 15.40| 21  | 2.879| 5   | 43.052| 13.519| 2.8316| 0.0009|
| 180  | 260 | 0.2 | 1.000| 0.000| 10.00| 0.080| 12.79| 18  | 4.174| 9   | 0.853| 7   | 11.762| 0   | 3.2227| 1.1239| 0.3808|
| 179  | 260 | 0.3 | 1.000| 0.000| 10.00| 0.080| 12.91| 64  | 4.228| 4   | 0.807| 0   | 11.380| 2   | 2.7695| 1.2195| 0.5468|
| 178  | 260 | 0.4 | 1.000| 0.000| 10.00| 0.080| 13.09| 45  | 4.264| 2   | 0.757| 4   | 11.048| 0   | 2.3576| 1.2899| 0.7073|
| 177  | 260 | 0.5 | 1.000| 0.000| 10.00| 0.080| 12.79| 18  | 4.174| 9   | 0.853| 7   | 11.627| 5   | 3.0665| 1.1568| 0.4239|
| 176  | 260 | 0.6 | 1.000| 0.000| 10.00| 0.080| 13.04| 99  | 4.102| 6   | 0.864| 6   | 11.727| 1   | 3.2006| 1.1217| 0.3722|
| 175  | 260 | 0.7 | 1.000| 0.000| 10.00| 0.080| 13.04| 99  | 4.102| 6   | 0.864| 6   | 11.739| 6   | 3.2848| 1.0866| 0.3308|
| 174  | 250 | 0.2 | 1.000| 0.000| 10.00| 0.080| 13.09| 45  | 4.264| 2   | 0.757| 4   | 11.048| 0   | 2.3576| 1.2899| 0.7073|
| 173  | 250 | 0.3 | 1.000| 0.000| 10.00| 0.080| 12.91| 64  | 4.228| 4   | 0.807| 0   | 11.380| 2   | 2.7695| 1.2195| 0.5468|
| 172  | 250 | 0.4 | 1.000| 0.000| 10.00| 0.080| 12.79| 18  | 4.174| 9   | 0.853| 7   | 11.654| 2   | 3.0664| 1.1553| 0.4371|
| 171  | 250 | 0.5 | 1.000| 0.000| 10.00| 0.080| 12.79| 18  | 4.174| 9   | 0.853| 7   | 11.762| 0   | 3.2227| 1.1239| 0.3808|
|   | 0   | 0   | 0   | 0   | 0   | 0   | 78  | 84  | 2   | 3   | 6   |   |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---|
| 186| 230 | 0.4 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 48.98| 91 | 16.06| 47 |
| 187| 240 | 0.6 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 47.05| 51 | 15.40| 21 |
| 188| 240 | 0.5 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 46.17| 78 | 15.34| 84 |
| 189| 240 | 0.4 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 48.98| 91 | 16.06| 47 |
| 190| 250 | 0.6 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 47.05| 51 | 15.40| 21 |
| 191| 250 | 0.5 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 46.17| 78 | 15.34| 84 |
| 192| 250 | 0.4 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 48.98| 91 | 16.06| 47 |
| 193| 260 | 0.6 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 47.05| 51 | 15.40| 21 |
| 194| 260 | 0.5 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 46.17| 78 | 15.34| 84 |
| 195| 260 | 0.4 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 48.98| 91 | 16.06| 47 |
| 196| 220 | 0.6 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 28.90| 52 | 8.083| 7  |
| 197| 220 | 0.5 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 30.54| 46 | 8.450| 3  |
| 198| 220 | 0.4 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 30.46| 74 | 8.530| 7  |
| 199| 230 | 0.6 | 1.000| 0   | 0.000| 0   | 5.000| 0   | 0.035| 0   | 28.90| 52 | 8.083| 7  |

Page 17 of 21
|    |     |     |     |     |     |     |     |
|----|-----|-----|-----|-----|-----|-----|-----|
| 200| 230 | 0.5 | 1.000| 0.000| 5.000| 0.035| 30.54 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 201| 230 | 0.4 | 1.000| 0.000| 5.000| 0.035| 30.46 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 202| 240 | 0.6 | 1.000| 0.000| 5.000| 0.035| 28.90 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 203| 240 | 0.5 | 1.000| 0.000| 5.000| 0.035| 30.54 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 204| 240 | 0.4 | 1.000| 0.000| 5.000| 0.035| 30.46 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 205| 250 | 0.6 | 1.000| 0.000| 5.000| 0.035| 28.90 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 206| 250 | 0.5 | 1.000| 0.000| 5.000| 0.035| 30.54 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 207| 250 | 0.4 | 1.000| 0.000| 5.000| 0.035| 30.46 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 208| 260 | 0.6 | 1.000| 0.000| 5.000| 0.035| 28.90 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 209| 260 | 0.5 | 1.000| 0.000| 5.000| 0.035| 30.54 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 210| 260 | 0.4 | 1.000| 0.000| 5.000| 0.035| 30.46 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 211| 220 | 0.6 | 1.000| 0.000| 5.000| 0.035| 20.35 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 212| 220 | 0.5 | 1.000| 0.000| 5.000| 0.035| 20.39 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 213| 220 | 0.4 | 1.000| 0.000| 5.000| 0.035| 20.45 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
| 214| 230 | 0.6 | 1.000| 0.000| 5.000| 0.035| 20.35 |
|    |     |     |     |     |     |     |     |
|    |     |     |     |     |     |     |     |
|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
|215 |230 |0.5 |1.000 |0.000 |5.000 |0.035 |0.000 |20.39 |61 |4.048 |9 |2.885 |5 |19.307 |9 |3.7063 |2.7876 |0.0001 |
|216 |230 |0.4 |1.000 |0.000 |5.000 |0.035 |0.000 |20.45 |05 |4.081 |4 |2.744 |2 |19.095 |7 |3.5794 |2.6585 |0.0002 |
|217 |240 |0.6 |1.000 |0.000 |5.000 |0.035 |0.000 |20.35 |88 |4.086 |5 |2.926 |2 |19.176 |3 |3.6972 |2.7619 |0.0002 |
|218 |240 |0.5 |1.000 |0.000 |5.000 |0.035 |0.000 |20.39 |61 |4.048 |9 |2.885 |5 |19.193 |9 |3.6563 |2.7724 |0.0004 |
|219 |240 |0.4 |1.000 |0.000 |5.000 |0.035 |0.000 |20.45 |05 |4.081 |4 |2.744 |2 |19.037 |2 |3.5557 |2.6410 |0.0007 |
|220 |250 |0.6 |1.000 |0.000 |5.000 |0.035 |0.000 |20.35 |88 |4.086 |5 |2.926 |2 |19.201 |3 |3.7195 |2.7526 |0.0007 |
|221 |250 |0.5 |1.000 |0.000 |5.000 |0.035 |0.000 |20.39 |61 |4.048 |9 |2.885 |5 |19.315 |4 |3.7010 |2.7806 |0.0009 |
|222 |250 |0.4 |1.000 |0.000 |5.000 |0.035 |0.000 |20.45 |05 |4.081 |4 |2.744 |2 |19.164 |6 |3.6435 |2.6339 |0.0013 |
|223 |260 |0.6 |1.000 |0.000 |5.000 |0.035 |0.000 |20.35 |88 |4.086 |5 |2.926 |2 |19.363 |0 |3.8358 |2.7351 |0.0011 |
|224 |260 |0.5 |1.000 |0.000 |5.000 |0.035 |0.000 |20.39 |61 |4.048 |9 |2.885 |5 |19.454 |5 |3.8211 |2.7394 |0.0014 |
|225 |260 |0.4 |1.000 |0.000 |5.000 |0.035 |0.000 |20.45 |05 |4.081 |4 |2.744 |2 |19.404 |3 |3.7903 |2.6187 |0.0019 |
|226 |220 |0.6 |1.000 |0.000 |5.000 |0.035 |0.000 |41.49 |47 |15.87 |93 |0.901 |6 |40.380 |8 |15.304 |9 |0.8354 |0.0001 |
|227 |220 |0.5 |1.000 |0.000 |5.000 |0.035 |0.000 |41.58 |78 |15.96 |64 |0.918 |4 |40.117 |6 |15.096 |2 |0.8783 |0.0003 |
|228 |220 |0.4 |1.000 |0.000 |5.000 |0.035 |0.000 |42.02 |74 |16.16 |33 |0.933 |9 |40.272 |1 |15.150 |0 |0.8998 |0.0007 |
| 229 | 230 | 0.6 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 41.49 | 47 | 15.87 | 93 | 0.901 | 6 | 39.922 | 4 | 15.044 | 9 | 0.8529 | 0.0006 |
|-----|-----|-----|-------|-------|-------|-------|---|-------|----|-------|---|-------|---|-------|----|-------|---|-------|---|
| 230 | 230 | 0.5 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 41.58 | 78 | 15.96 | 64 | 0.918 | 4 | 39.452 | 1 | 14.780 | 5 | 0.8975 | 0.0011 |
| 231 | 230 | 0.4 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 42.02 | 74 | 16.16 | 33 | 0.933 | 9 | 39.502 | 1 | 14.689 | 2 | 0.9109 | 0.0022 |
| 232 | 240 | 0.6 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 41.49 | 78 | 15.87 | 93 | 0.901 | 6 | 39.922 | 4 | 14.580 | 1 | 0.8706 | 0.0017 |
| 233 | 240 | 0.5 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 41.58 | 78 | 15.96 | 64 | 0.918 | 4 | 38.648 | 6 | 14.328 | 1 | 0.9101 | 0.0026 |
| 234 | 240 | 0.4 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 42.02 | 74 | 16.16 | 33 | 0.933 | 9 | 38.842 | 8 | 14.242 | 1 | 0.9441 | 0.0045 |
| 235 | 250 | 0.6 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 41.49 | 78 | 15.87 | 93 | 0.901 | 6 | 38.425 | 8 | 14.200 | 2 | 0.8956 | 0.0039 |
| 236 | 250 | 0.5 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 41.58 | 78 | 15.96 | 64 | 0.918 | 4 | 38.067 | 6 | 13.984 | 0 | 0.9377 | 0.0051 |
| 237 | 250 | 0.4 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 42.02 | 74 | 16.16 | 33 | 0.933 | 9 | 38.483 | 5 | 13.980 | 6 | 0.9656 | 0.0075 |
| 238 | 260 | 0.6 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 41.49 | 47 | 15.87 | 93 | 0.901 | 6 | 38.111 | 8 | 13.956 | 2 | 0.9152 | 0.0058 |
| 239 | 260 | 0.5 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 41.58 | 78 | 15.96 | 64 | 0.918 | 4 | 37.726 | 1 | 13.781 | 3 | 0.9699 | 0.0093 |
| 240 | 260 | 0.4 | 1.000 | 0.000 | 5.000 | 0.035 | 0 | 42.02 | 74 | 16.16 | 33 | 0.933 | 9 | 38.454 | 8 | 13.879 | 8 | 0.9923 | 0.0136 |
Section 4.4 Optimization results

The reaction rate profiles for optimization cases A2, B1 and B2, along with the respective reference cases are presented here (Figures 4 to 6) complementary to the results in Section 4.4. At optimal conditions, increased reaction rates along the reactor coordinate can be observed in each case. These results resemble the ones obtained for optimization case A1, which were previously discussed in Section 4.4.1.1.

Figure 4.

Example A - Modified reaction rates

Solid lines: reference case
Dashed lines: optimization case A2.

Conditions reported in Table 5 and Table 6. $L_{\text{bed}} = 5.5$ cm.

Figure 5.

Example B - Modified reaction rates

Solid lines: reference case
Dashed lines: optimization case B1.

Conditions reported in Table 5 and Table 7. $L_{\text{bed}} = 8$ cm.

Figure 6.

Example B - Modified reaction rates

Solid lines: reference case
Dashed lines: optimization case B2.

Conditions reported in Table 5 and Table 7. $L_{\text{bed}} = 8$ cm.