Supplementary Material

* The model developed:

The pickle file for the XGB model of CO2 fugacity coefficient can be found from author’s [github](https://github.com/Rupom-Bhattacherjee/Modeling-CO2-Fugacity-Coefficient/blob/main/XGBModel_phi_rf.sav) link.

* Codes required to make prediction:

To estimate the log of fugacity coefficient (the value commonly required in the application of fugacity coefficient, such as for solubility estimation), following lines of code can be used:

*import pickle*

*import math*

*phi\_from\_pickle = pickle.load(open(r 'C:\XGBModel\_phi\_rf.sav', 'rb')) # replace the path with the file path to the pickle file*

*math.log(phi\_from\_pickle.predict([[T,P]])[0]) # Insert T in °C and P in bar*

* Scored data:

The scored data with fugacity and CO2 solubility is uploaded as separate files, but also available in github.

The original 640 datapoints used in training and testing the fugacity model are listed in the following table:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Data Set** | **T/C** | **P/bar** | **CO2 fugacity coefficient** | **Data Source** |
| Train | 0 | 1 | 0.993 | Angus et al. 1976 |
| Train | 40 | 1 | 0.996 | Angus et al. 1976 |
| Train | 60 | 1 | 0.996 | Angus et al. 1976 |
| Train | 80 | 1 | 0.997 | Angus et al. 1976 |
| Train | 120 | 1 | 0.998 | Angus et al. 1976 |
| Train | 200 | 1 | 0.999 | Angus et al. 1976 |
| Train | 545 | 1 | 1.000 | Angus et al. 1976 |
| Train | 620 | 1 | 1.000 | Angus et al. 1976 |
| Train | 820 | 1 | 1.000 | Angus et al. 1976 |
| Train | 0 | 50 | 0.657 | Angus et al. 1976 |
| Train | 40 | 50 | 0.790 | Angus et al. 1976 |
| Train | 60 | 50 | 0.834 | Angus et al. 1976 |
| Test | 80 | 50 | 0.861 | Angus et al. 1976 |
| Test | 120 | 50 | 0.896 | Angus et al. 1976 |
| Train | 200 | 50 | 0.958 | Angus et al. 1976 |
| Test | 220 | 50 | 0.959 | Angus et al. 1976 |
| Test | 320 | 50 | 0.988 | Angus et al. 1976 |
| Test | 345 | 50 | 0.995 | Angus et al. 1976 |
| Test | 460 | 50 | 1.001 | Angus et al. 1976 |
| Train | 545 | 50 | 1.006 | Angus et al. 1976 |
| Test | 620 | 50 | 1.007 | Angus et al. 1976 |
| Test | 820 | 50 | 1.010 | Angus et al. 1976 |
| Train | 0 | 100 | 0.315 | Angus et al. 1976 |
| Train | 40 | 100 | 0.577 | Angus et al. 1976 |
| Train | 60 | 100 | 0.673 | Angus et al. 1976 |
| Test | 80 | 100 | 0.730 | Angus et al. 1976 |
| Test | 120 | 100 | 0.800 | Angus et al. 1976 |
| Test | 220 | 100 | 0.925 | Angus et al. 1976 |
| Test | 320 | 100 | 0.976 | Angus et al. 1976 |
| Test | 345 | 100 | 0.990 | Angus et al. 1976 |
| Test | 460 | 100 | 1.007 | Angus et al. 1976 |
| Train | 500 | 100 | 1.010 | Rhyzenko, 1971 |
| Test | 620 | 100 | 1.018 | Angus et al. 1976 |
| Test | 820 | 100 | 1.021 | Angus et al. 1976 |
| Test | 1000 | 100 | 1.027 | Rhyzenko, 1971 |
| Test | 1000 | 100 | 1.030 | Rhyzenko, 1971 |
| Train | 0 | 200 | 0.192 | Angus et al. 1976 |
| Train | 40 | 200 | 0.360 | Angus et al. 1976 |
| Test | 80 | 200 | 0.533 | Angus et al. 1976 |
| Test | 120 | 200 | 0.647 | Angus et al. 1976 |
| Train | 200 | 200 | 0.853 | Angus et al. 1976 |
| Test | 220 | 200 | 0.861 | Angus et al. 1976 |
| Test | 320 | 200 | 0.957 | Angus et al. 1976 |
| Test | 345 | 200 | 0.983 | Angus et al. 1976 |
| Test | 460 | 200 | 1.009 | Angus et al. 1976 |
| Train | 500 | 200 | 1.023 | Rhyzenko, 1971 |
| Test | 620 | 200 | 1.032 | Angus et al. 1976 |
| Train | 800 | 200 | 1.042 | Rhyzenko, 1971 |
| Test | 820 | 200 | 1.043 | Angus et al. 1976 |
| Test | 1000 | 200 | 1.053 | Rhyzenko, 1971 |
| Test | 1000 | 200 | 1.055 | Rhyzenko, 1971 |
| Train | 0 | 300 | 0.154 | Angus et al. 1976 |
| Train | 40 | 300 | 0.291 | Angus et al. 1976 |
| Train | 60 | 300 | 0.370 | Angus et al. 1976 |
| Test | 80 | 300 | 0.441 | Angus et al. 1976 |
| Test | 120 | 300 | 0.554 | Angus et al. 1976 |
| Train | 200 | 300 | 0.806 | Angus et al. 1976 |
| Test | 220 | 300 | 0.813 | Angus et al. 1976 |
| Test | 320 | 300 | 0.949 | Angus et al. 1976 |
| Test | 345 | 300 | 0.976 | Angus et al. 1976 |
| Train | 400 | 300 | 1.007 | Ryzhenko, 1971 |
| Train | 500 | 300 | 1.010 | Ryzhenko, 1971 |
| Train | 600 | 300 | 1.055 | Ryzhenko, 1971 |
| Train | 800 | 300 | 1.065 | Ryzhenko, 1971 |
| Train | 1000 | 300 | 1.065 | Ryzhenko, 1971 |
| Train | 0 | 400 | 0.138 | Angus et al. 1976 |
| Train | 40 | 400 | 0.262 | Angus et al. 1976 |
| Train | 60 | 400 | 0.334 | Angus et al. 1976 |
| Train | 200 | 400 | 0.778 | Angus et al. 1976 |
| Test | 420 | 400 | 1.016 | Angus et al. 1976 |
| Test | 460 | 400 | 1.040 | Angus et al. 1976 |
| Train | 500 | 400 | 1.058 | Ryzhenko, 1971 |
| Test | 620 | 400 | 1.080 | Angus et al. 1976 |
| Test | 820 | 400 | 1.097 | Angus et al. 1976 |
| Test | 1000 | 400 | 1.099 | Ryzhenko, 1971 |
| Test | 1000 | 400 | 1.096 | Ryzhenko, 1971 |
| Train | 0 | 500 | 0.133 | Angus et al. 1976 |
| Train | 40 | 500 | 0.249 | Angus et al. 1976 |
| Train | 60 | 500 | 0.318 | Angus et al. 1976 |
| Test | 80 | 500 | 0.382 | Angus et al. 1976 |
| Test | 120 | 500 | 0.487 | Angus et al. 1976 |
| Train | 200 | 500 | 0.766 | Angus et al. 1976 |
| Test | 220 | 500 | 0.777 | Angus et al. 1976 |
| Test | 320 | 500 | 0.942 | Angus et al. 1976 |
| Test | 345 | 500 | 0.969 | Angus et al. 1976 |
| Train | 400 | 500 | 1.035 | Ryzhenko, 1971 |
| Train | 500 | 500 | 1.081 | Ryzhenko, 1971 |
| Train | 600 | 500 | 1.103 | Ryzhenko, 1971 |
| Train | 800 | 500 | 1.116 | Ryzhenko, 1971 |
| Train | 1000 | 500 | 1.113 | Ryzhenko, 1971 |
| Train | 0 | 600 | 0.132 | Angus et al. 1976 |
| Train | 40 | 600 | 0.246 | Angus et al. 1976 |
| Train | 60 | 600 | 0.313 | Angus et al. 1976 |
| Train | 200 | 600 | 0.766 | Angus et al. 1976 |
| Test | 420 | 600 | 1.058 | Angus et al. 1976 |
| Test | 460 | 600 | 1.089 | Angus et al. 1976 |
| Train | 500 | 600 | 1.106 | Ryzhenko, 1971 |
| Train | 545 | 600 | 1.120 | Angus et al. 1976 |
| Test | 620 | 600 | 1.137 | Angus et al. 1976 |
| Test | 820 | 600 | 1.157 | Angus et al. 1976 |
| Test | 1000 | 600 | 1.151 | Ryzhenko, 1971 |
| Test | 1000 | 600 | 1.149 | Ryzhenko, 1971 |
| Train | 400 | 700 | 1.000 | Ryzhenko, 1971 |
| Train | 500 | 700 | 1.081 | Ryzhenko, 1971 |
| Train | 600 | 700 | 1.135 | Ryzhenko, 1971 |
| Train | 800 | 700 | 1.161 | Ryzhenko, 1971 |
| Train | 1000 | 700 | 1.166 | Ryzhenko, 1971 |
| Train | 0 | 800 | 0.138 | Angus et al. 1976 |
| Train | 40 | 800 | 0.254 | Angus et al. 1976 |
| Train | 60 | 800 | 0.324 | Angus et al. 1976 |
| Train | 200 | 800 | 0.793 | Angus et al. 1976 |
| Test | 410 | 800 | 1.115 | Ryzhenko, 1971 |
| Test | 420 | 800 | 1.115 | Angus et al. 1976 |
| Test | 450 | 800 | 1.153 | Ryzhenko, 1971 |
| Test | 460 | 800 | 1.154 | Angus et al. 1976 |
| Train | 500 | 800 | 1.167 | Ryzhenko, 1971 |
| Train | 545 | 800 | 1.182 | Angus et al. 1976 |
| Test | 600 | 800 | 1.196 | Ryzhenko, 1971 |
| Test | 620 | 800 | 1.197 | Angus et al. 1976 |
| Test | 800 | 800 | 1.213 | Ryzhenko, 1971 |
| Test | 820 | 800 | 1.214 | Angus et al. 1976 |
| Test | 1000 | 800 | 1.204 | Ryzhenko, 1971 |
| Train | 400 | 900 | 1.145 | Ryzhenko, 1971 |
| Train | 500 | 900 | 1.203 | Ryzhenko, 1971 |
| Train | 600 | 900 | 1.228 | Ryzhenko, 1971 |
| Train | 800 | 900 | 1.236 | Ryzhenko, 1971 |
| Train | 1000 | 900 | 1.223 | Ryzhenko, 1971 |
| Train | 0 | 1000 | 0.154 | Angus et al. 1976 |
| Train | 40 | 1000 | 0.279 | Angus et al. 1976 |
| Train | 60 | 1000 | 0.350 | Angus et al. 1976 |
| Train | 80 | 1000 | 0.428 | Angus et al. 1976 |
| Train | 120 | 1000 | 0.580 | Angus et al. 1976 |
| Train | 200 | 1000 | 0.845 | Angus et al. 1976 |
| Test | 400 | 1000 | 1.190 | Ryzhenko, 1971 |
| Test | 450 | 1000 | 1.230 | Ryzhenko, 1971 |
| Train | 500 | 1000 | 1.242 | Ryzhenko, 1971 |
| Test | 600 | 1000 | 1.272 | Ryzhenko, 1971 |
| Test | 800 | 1000 | 1.281 | Ryzhenko, 1971 |
| Train | 820 | 1000 | 1.269 | Angus et al. 1976 |
| Test | 1000 | 1000 | 1.263 | Ryzhenko, 1971 |
| Train | 0 | 1040 | 0.158 | Duan et al., 1992 |
| Train | 40 | 1040 | 0.286 | Duan et al., 1992 |
| Train | 60 | 1040 | 0.357 | Duan et al., 1992 |
| Train | 80 | 1040 | 0.437 | Duan et al., 1992 |
| Train | 120 | 1040 | 0.592 | Duan et al., 1992 |
| Train | 200 | 1040 | 0.860 | Duan et al., 1992 |
| Train | 220 | 1040 | 0.914 | Duan et al., 1992 |
| Train | 320 | 1040 | 1.112 | Duan et al., 1992 |
| Train | 345 | 1040 | 1.145 | Duan et al., 1992 |
| Train | 400 | 1040 | 1.201 | Duan et al., 1992 |
| Train | 420 | 1040 | 1.216 | Duan et al., 1992 |
| Train | 450 | 1040 | 1.235 | Duan et al., 1992 |
| Train | 460 | 1040 | 1.241 | Duan et al., 1992 |
| Train | 500 | 1040 | 1.258 | Duan et al., 1992 |
| Train | 545 | 1040 | 1.272 | Duan et al., 1992 |
| Train | 600 | 1040 | 1.282 | Duan et al., 1992 |
| Train | 620 | 1040 | 1.285 | Duan et al., 1992 |
| Train | 800 | 1040 | 1.285 | Duan et al., 1992 |
| Train | 820 | 1040 | 1.283 | Duan et al., 1992 |
| Train | 1000 | 1040 | 1.266 | Duan et al., 1992 |
| Train | 0 | 1080 | 0.163 | Duan et al., 1992 |
| Train | 40 | 1080 | 0.293 | Duan et al., 1992 |
| Train | 60 | 1080 | 0.365 | Duan et al., 1992 |
| Train | 80 | 1080 | 0.445 | Duan et al., 1992 |
| Train | 120 | 1080 | 0.601 | Duan et al., 1992 |
| Train | 200 | 1080 | 0.874 | Duan et al., 1992 |
| Train | 220 | 1080 | 0.928 | Duan et al., 1992 |
| Train | 320 | 1080 | 1.129 | Duan et al., 1992 |
| Train | 345 | 1080 | 1.163 | Duan et al., 1992 |
| Train | 400 | 1080 | 1.218 | Duan et al., 1992 |
| Train | 420 | 1080 | 1.234 | Duan et al., 1992 |
| Train | 450 | 1080 | 1.253 | Duan et al., 1992 |
| Train | 460 | 1080 | 1.258 | Duan et al., 1992 |
| Train | 500 | 1080 | 1.275 | Duan et al., 1992 |
| Train | 545 | 1080 | 1.289 | Duan et al., 1992 |
| Train | 600 | 1080 | 1.299 | Duan et al., 1992 |
| Train | 620 | 1080 | 1.301 | Duan et al., 1992 |
| Train | 800 | 1080 | 1.299 | Duan et al., 1992 |
| Train | 820 | 1080 | 1.298 | Duan et al., 1992 |
| Train | 1000 | 1080 | 1.279 | Duan et al., 1992 |
| Train | 0 | 1120 | 0.168 | Duan et al., 1992 |
| Train | 40 | 1120 | 0.301 | Duan et al., 1992 |
| Train | 60 | 1120 | 0.374 | Duan et al., 1992 |
| Train | 80 | 1120 | 0.454 | Duan et al., 1992 |
| Train | 120 | 1120 | 0.612 | Duan et al., 1992 |
| Train | 200 | 1120 | 0.888 | Duan et al., 1992 |
| Train | 220 | 1120 | 0.944 | Duan et al., 1992 |
| Train | 320 | 1120 | 1.147 | Duan et al., 1992 |
| Train | 345 | 1120 | 1.180 | Duan et al., 1992 |
| Train | 400 | 1120 | 1.236 | Duan et al., 1992 |
| Train | 420 | 1120 | 1.251 | Duan et al., 1992 |
| Train | 450 | 1120 | 1.270 | Duan et al., 1992 |
| Train | 460 | 1120 | 1.275 | Duan et al., 1992 |
| Train | 500 | 1120 | 1.293 | Duan et al., 1992 |
| Train | 545 | 1120 | 1.306 | Duan et al., 1992 |
| Train | 600 | 1120 | 1.315 | Duan et al., 1992 |
| Train | 620 | 1120 | 1.317 | Duan et al., 1992 |
| Train | 800 | 1120 | 1.314 | Duan et al., 1992 |
| Train | 820 | 1120 | 1.312 | Duan et al., 1992 |
| Train | 1000 | 1120 | 1.292 | Duan et al., 1992 |
| Train | 0 | 1160 | 0.173 | Duan et al., 1992 |
| Train | 40 | 1160 | 0.308 | Duan et al., 1992 |
| Train | 60 | 1160 | 0.383 | Duan et al., 1992 |
| Train | 80 | 1160 | 0.463 | Duan et al., 1992 |
| Train | 120 | 1160 | 0.624 | Duan et al., 1992 |
| Train | 200 | 1160 | 0.904 | Duan et al., 1992 |
| Train | 220 | 1160 | 0.962 | Duan et al., 1992 |
| Train | 320 | 1160 | 1.164 | Duan et al., 1992 |
| Train | 345 | 1160 | 1.198 | Duan et al., 1992 |
| Train | 400 | 1160 | 1.254 | Duan et al., 1992 |
| Train | 420 | 1160 | 1.270 | Duan et al., 1992 |
| Train | 450 | 1160 | 1.289 | Duan et al., 1992 |
| Train | 460 | 1160 | 1.294 | Duan et al., 1992 |
| Train | 500 | 1160 | 1.311 | Duan et al., 1992 |
| Train | 545 | 1160 | 1.324 | Duan et al., 1992 |
| Train | 600 | 1160 | 1.332 | Duan et al., 1992 |
| Train | 620 | 1160 | 1.334 | Duan et al., 1992 |
| Train | 800 | 1160 | 1.329 | Duan et al., 1992 |
| Train | 820 | 1160 | 1.327 | Duan et al., 1992 |
| Train | 1000 | 1160 | 1.305 | Duan et al., 1992 |
| Train | 0 | 1200 | 0.179 | Duan et al., 1992 |
| Train | 40 | 1200 | 0.315 | Duan et al., 1992 |
| Train | 60 | 1200 | 0.393 | Duan et al., 1992 |
| Train | 80 | 1200 | 0.474 | Duan et al., 1992 |
| Train | 120 | 1200 | 0.637 | Duan et al., 1992 |
| Train | 200 | 1200 | 0.921 | Duan et al., 1992 |
| Train | 220 | 1200 | 0.979 | Duan et al., 1992 |
| Train | 320 | 1200 | 1.183 | Duan et al., 1992 |
| Train | 345 | 1200 | 1.218 | Duan et al., 1992 |
| Train | 400 | 1200 | 1.273 | Duan et al., 1992 |
| Train | 420 | 1200 | 1.289 | Duan et al., 1992 |
| Train | 450 | 1200 | 1.307 | Duan et al., 1992 |
| Train | 460 | 1200 | 1.313 | Duan et al., 1992 |
| Train | 500 | 1200 | 1.330 | Duan et al., 1992 |
| Train | 545 | 1200 | 1.342 | Duan et al., 1992 |
| Train | 600 | 1200 | 1.350 | Duan et al., 1992 |
| Train | 620 | 1200 | 1.351 | Duan et al., 1992 |
| Train | 800 | 1200 | 1.344 | Duan et al., 1992 |
| Train | 820 | 1200 | 1.342 | Duan et al., 1992 |
| Train | 1000 | 1200 | 1.318 | Duan et al., 1992 |
| Train | 0 | 1240 | 0.185 | Duan et al., 1992 |
| Train | 40 | 1240 | 0.323 | Duan et al., 1992 |
| Train | 60 | 1240 | 0.403 | Duan et al., 1992 |
| Train | 80 | 1240 | 0.485 | Duan et al., 1992 |
| Train | 120 | 1240 | 0.651 | Duan et al., 1992 |
| Train | 200 | 1240 | 0.939 | Duan et al., 1992 |
| Train | 220 | 1240 | 0.996 | Duan et al., 1992 |
| Train | 320 | 1240 | 1.204 | Duan et al., 1992 |
| Train | 345 | 1240 | 1.237 | Duan et al., 1992 |
| Train | 400 | 1240 | 1.294 | Duan et al., 1992 |
| Train | 420 | 1240 | 1.308 | Duan et al., 1992 |
| Train | 450 | 1240 | 1.327 | Duan et al., 1992 |
| Train | 460 | 1240 | 1.332 | Duan et al., 1992 |
| Train | 500 | 1240 | 1.349 | Duan et al., 1992 |
| Train | 545 | 1240 | 1.360 | Duan et al., 1992 |
| Train | 600 | 1240 | 1.368 | Duan et al., 1992 |
| Train | 620 | 1240 | 1.370 | Duan et al., 1992 |
| Train | 800 | 1240 | 1.360 | Duan et al., 1992 |
| Train | 820 | 1240 | 1.358 | Duan et al., 1992 |
| Train | 1000 | 1240 | 1.332 | Duan et al., 1992 |
| Train | 0 | 1280 | 0.191 | Duan et al., 1992 |
| Train | 40 | 1280 | 0.332 | Duan et al., 1992 |
| Train | 60 | 1280 | 0.415 | Duan et al., 1992 |
| Train | 80 | 1280 | 0.497 | Duan et al., 1992 |
| Train | 120 | 1280 | 0.666 | Duan et al., 1992 |
| Train | 200 | 1280 | 0.958 | Duan et al., 1992 |
| Train | 220 | 1280 | 1.014 | Duan et al., 1992 |
| Train | 320 | 1280 | 1.224 | Duan et al., 1992 |
| Train | 345 | 1280 | 1.257 | Duan et al., 1992 |
| Train | 400 | 1280 | 1.314 | Duan et al., 1992 |
| Train | 420 | 1280 | 1.329 | Duan et al., 1992 |
| Train | 450 | 1280 | 1.347 | Duan et al., 1992 |
| Train | 460 | 1280 | 1.353 | Duan et al., 1992 |
| Train | 500 | 1280 | 1.369 | Duan et al., 1992 |
| Train | 545 | 1280 | 1.380 | Duan et al., 1992 |
| Train | 600 | 1280 | 1.387 | Duan et al., 1992 |
| Train | 620 | 1280 | 1.387 | Duan et al., 1992 |
| Train | 800 | 1280 | 1.376 | Duan et al., 1992 |
| Train | 820 | 1280 | 1.373 | Duan et al., 1992 |
| Train | 1000 | 1280 | 1.345 | Duan et al., 1992 |
| Train | 0 | 1320 | 0.198 | Duan et al., 1992 |
| Train | 40 | 1320 | 0.341 | Duan et al., 1992 |
| Train | 60 | 1320 | 0.427 | Duan et al., 1992 |
| Train | 80 | 1320 | 0.509 | Duan et al., 1992 |
| Train | 120 | 1320 | 0.682 | Duan et al., 1992 |
| Train | 200 | 1320 | 0.977 | Duan et al., 1992 |
| Train | 220 | 1320 | 1.034 | Duan et al., 1992 |
| Train | 320 | 1320 | 1.244 | Duan et al., 1992 |
| Train | 345 | 1320 | 1.279 | Duan et al., 1992 |
| Train | 400 | 1320 | 1.335 | Duan et al., 1992 |
| Train | 420 | 1320 | 1.350 | Duan et al., 1992 |
| Train | 450 | 1320 | 1.368 | Duan et al., 1992 |
| Train | 460 | 1320 | 1.373 | Duan et al., 1992 |
| Train | 500 | 1320 | 1.388 | Duan et al., 1992 |
| Train | 545 | 1320 | 1.399 | Duan et al., 1992 |
| Train | 600 | 1320 | 1.406 | Duan et al., 1992 |
| Train | 620 | 1320 | 1.406 | Duan et al., 1992 |
| Train | 800 | 1320 | 1.392 | Duan et al., 1992 |
| Train | 820 | 1320 | 1.389 | Duan et al., 1992 |
| Train | 1000 | 1320 | 1.359 | Duan et al., 1992 |
| Train | 0 | 1360 | 0.206 | Duan et al., 1992 |
| Train | 40 | 1360 | 0.350 | Duan et al., 1992 |
| Train | 60 | 1360 | 0.439 | Duan et al., 1992 |
| Train | 80 | 1360 | 0.523 | Duan et al., 1992 |
| Train | 120 | 1360 | 0.699 | Duan et al., 1992 |
| Train | 200 | 1360 | 0.996 | Duan et al., 1992 |
| Train | 220 | 1360 | 1.055 | Duan et al., 1992 |
| Train | 320 | 1360 | 1.266 | Duan et al., 1992 |
| Train | 345 | 1360 | 1.302 | Duan et al., 1992 |
| Train | 400 | 1360 | 1.357 | Duan et al., 1992 |
| Train | 420 | 1360 | 1.371 | Duan et al., 1992 |
| Train | 450 | 1360 | 1.389 | Duan et al., 1992 |
| Train | 460 | 1360 | 1.394 | Duan et al., 1992 |
| Train | 500 | 1360 | 1.409 | Duan et al., 1992 |
| Train | 545 | 1360 | 1.420 | Duan et al., 1992 |
| Train | 600 | 1360 | 1.425 | Duan et al., 1992 |
| Train | 620 | 1360 | 1.425 | Duan et al., 1992 |
| Train | 800 | 1360 | 1.409 | Duan et al., 1992 |
| Train | 820 | 1360 | 1.406 | Duan et al., 1992 |
| Train | 1000 | 1360 | 1.373 | Duan et al., 1992 |
| Train | 0 | 1400 | 0.213 | Duan et al., 1992 |
| Train | 40 | 1400 | 0.361 | Duan et al., 1992 |
| Train | 60 | 1400 | 0.451 | Duan et al., 1992 |
| Train | 80 | 1400 | 0.537 | Duan et al., 1992 |
| Train | 120 | 1400 | 0.717 | Duan et al., 1992 |
| Train | 200 | 1400 | 1.016 | Duan et al., 1992 |
| Train | 220 | 1400 | 1.078 | Duan et al., 1992 |
| Train | 320 | 1400 | 1.290 | Duan et al., 1992 |
| Train | 345 | 1400 | 1.324 | Duan et al., 1992 |
| Train | 400 | 1400 | 1.380 | Duan et al., 1992 |
| Train | 420 | 1400 | 1.393 | Duan et al., 1992 |
| Train | 450 | 1400 | 1.412 | Duan et al., 1992 |
| Train | 460 | 1400 | 1.416 | Duan et al., 1992 |
| Train | 500 | 1400 | 1.431 | Duan et al., 1992 |
| Train | 545 | 1400 | 1.441 | Duan et al., 1992 |
| Train | 600 | 1400 | 1.445 | Duan et al., 1992 |
| Train | 620 | 1400 | 1.445 | Duan et al., 1992 |
| Train | 800 | 1400 | 1.426 | Duan et al., 1992 |
| Train | 820 | 1400 | 1.422 | Duan et al., 1992 |
| Train | 1000 | 1400 | 1.388 | Duan et al., 1992 |
| Train | 0 | 1440 | 0.220 | Duan et al., 1992 |
| Train | 40 | 1440 | 0.372 | Duan et al., 1992 |
| Train | 60 | 1440 | 0.463 | Duan et al., 1992 |
| Train | 80 | 1440 | 0.552 | Duan et al., 1992 |
| Train | 120 | 1440 | 0.737 | Duan et al., 1992 |
| Train | 200 | 1440 | 1.037 | Duan et al., 1992 |
| Train | 220 | 1440 | 1.101 | Duan et al., 1992 |
| Train | 320 | 1440 | 1.314 | Duan et al., 1992 |
| Train | 345 | 1440 | 1.347 | Duan et al., 1992 |
| Train | 400 | 1440 | 1.402 | Duan et al., 1992 |
| Train | 420 | 1440 | 1.417 | Duan et al., 1992 |
| Train | 450 | 1440 | 1.433 | Duan et al., 1992 |
| Train | 460 | 1440 | 1.439 | Duan et al., 1992 |
| Train | 500 | 1440 | 1.452 | Duan et al., 1992 |
| Train | 545 | 1440 | 1.461 | Duan et al., 1992 |
| Train | 600 | 1440 | 1.465 | Duan et al., 1992 |
| Train | 620 | 1440 | 1.465 | Duan et al., 1992 |
| Train | 800 | 1440 | 1.443 | Duan et al., 1992 |
| Train | 820 | 1440 | 1.439 | Duan et al., 1992 |
| Train | 1000 | 1440 | 1.403 | Duan et al., 1992 |
| Train | 0 | 1480 | 0.227 | Duan et al., 1992 |
| Train | 40 | 1480 | 0.383 | Duan et al., 1992 |
| Train | 60 | 1480 | 0.476 | Duan et al., 1992 |
| Train | 80 | 1480 | 0.569 | Duan et al., 1992 |
| Train | 120 | 1480 | 0.753 | Duan et al., 1992 |
| Train | 200 | 1480 | 1.060 | Duan et al., 1992 |
| Train | 220 | 1480 | 1.122 | Duan et al., 1992 |
| Train | 320 | 1480 | 1.338 | Duan et al., 1992 |
| Train | 345 | 1480 | 1.371 | Duan et al., 1992 |
| Train | 400 | 1480 | 1.425 | Duan et al., 1992 |
| Train | 420 | 1480 | 1.440 | Duan et al., 1992 |
| Train | 450 | 1480 | 1.456 | Duan et al., 1992 |
| Train | 460 | 1480 | 1.461 | Duan et al., 1992 |
| Train | 500 | 1480 | 1.475 | Duan et al., 1992 |
| Train | 545 | 1480 | 1.483 | Duan et al., 1992 |
| Train | 600 | 1480 | 1.486 | Duan et al., 1992 |
| Train | 620 | 1480 | 1.485 | Duan et al., 1992 |
| Train | 800 | 1480 | 1.461 | Duan et al., 1992 |
| Train | 820 | 1480 | 1.456 | Duan et al., 1992 |
| Train | 1000 | 1480 | 1.417 | Duan et al., 1992 |
| Train | 0 | 1520 | 0.235 | Duan et al., 1992 |
| Train | 40 | 1520 | 0.395 | Duan et al., 1992 |
| Train | 60 | 1520 | 0.489 | Duan et al., 1992 |
| Train | 80 | 1520 | 0.585 | Duan et al., 1992 |
| Train | 120 | 1520 | 0.771 | Duan et al., 1992 |
| Train | 200 | 1520 | 1.083 | Duan et al., 1992 |
| Train | 220 | 1520 | 1.145 | Duan et al., 1992 |
| Train | 320 | 1520 | 1.362 | Duan et al., 1992 |
| Train | 345 | 1520 | 1.397 | Duan et al., 1992 |
| Train | 400 | 1520 | 1.450 | Duan et al., 1992 |
| Train | 420 | 1520 | 1.464 | Duan et al., 1992 |
| Train | 450 | 1520 | 1.481 | Duan et al., 1992 |
| Train | 460 | 1520 | 1.485 | Duan et al., 1992 |
| Train | 500 | 1520 | 1.498 | Duan et al., 1992 |
| Train | 545 | 1520 | 1.506 | Duan et al., 1992 |
| Train | 600 | 1520 | 1.508 | Duan et al., 1992 |
| Train | 620 | 1520 | 1.506 | Duan et al., 1992 |
| Train | 800 | 1520 | 1.478 | Duan et al., 1992 |
| Train | 820 | 1520 | 1.474 | Duan et al., 1992 |
| Train | 1000 | 1520 | 1.433 | Duan et al., 1992 |
| Train | 0 | 1560 | 0.243 | Duan et al., 1992 |
| Train | 40 | 1560 | 0.408 | Duan et al., 1992 |
| Train | 60 | 1560 | 0.503 | Duan et al., 1992 |
| Train | 80 | 1560 | 0.603 | Duan et al., 1992 |
| Train | 120 | 1560 | 0.790 | Duan et al., 1992 |
| Train | 200 | 1560 | 1.108 | Duan et al., 1992 |
| Train | 220 | 1560 | 1.169 | Duan et al., 1992 |
| Train | 320 | 1560 | 1.387 | Duan et al., 1992 |
| Train | 345 | 1560 | 1.424 | Duan et al., 1992 |
| Train | 400 | 1560 | 1.477 | Duan et al., 1992 |
| Train | 420 | 1560 | 1.489 | Duan et al., 1992 |
| Train | 450 | 1560 | 1.506 | Duan et al., 1992 |
| Train | 460 | 1560 | 1.510 | Duan et al., 1992 |
| Train | 500 | 1560 | 1.522 | Duan et al., 1992 |
| Train | 545 | 1560 | 1.528 | Duan et al., 1992 |
| Train | 600 | 1560 | 1.528 | Duan et al., 1992 |
| Train | 620 | 1560 | 1.528 | Duan et al., 1992 |
| Train | 800 | 1560 | 1.496 | Duan et al., 1992 |
| Train | 820 | 1560 | 1.491 | Duan et al., 1992 |
| Train | 1000 | 1560 | 1.447 | Duan et al., 1992 |
| Train | 0 | 1600 | 0.252 | Duan et al., 1992 |
| Train | 40 | 1600 | 0.422 | Duan et al., 1992 |
| Train | 60 | 1600 | 0.518 | Duan et al., 1992 |
| Train | 80 | 1600 | 0.622 | Duan et al., 1992 |
| Train | 120 | 1600 | 0.810 | Duan et al., 1992 |
| Train | 200 | 1600 | 1.135 | Duan et al., 1992 |
| Train | 220 | 1600 | 1.195 | Duan et al., 1992 |
| Train | 320 | 1600 | 1.414 | Duan et al., 1992 |
| Train | 345 | 1600 | 1.448 | Duan et al., 1992 |
| Train | 400 | 1600 | 1.502 | Duan et al., 1992 |
| Train | 420 | 1600 | 1.515 | Duan et al., 1992 |
| Train | 450 | 1600 | 1.530 | Duan et al., 1992 |
| Train | 460 | 1600 | 1.535 | Duan et al., 1992 |
| Train | 500 | 1600 | 1.545 | Duan et al., 1992 |
| Train | 545 | 1600 | 1.551 | Duan et al., 1992 |
| Train | 600 | 1600 | 1.550 | Duan et al., 1992 |
| Train | 620 | 1600 | 1.549 | Duan et al., 1992 |
| Train | 800 | 1600 | 1.515 | Duan et al., 1992 |
| Train | 820 | 1600 | 1.510 | Duan et al., 1992 |
| Train | 1000 | 1600 | 1.463 | Duan et al., 1992 |
| Train | 0 | 1640 | 0.261 | Duan et al., 1992 |
| Train | 40 | 1640 | 0.436 | Duan et al., 1992 |
| Train | 60 | 1640 | 0.534 | Duan et al., 1992 |
| Train | 80 | 1640 | 0.642 | Duan et al., 1992 |
| Train | 120 | 1640 | 0.831 | Duan et al., 1992 |
| Train | 200 | 1640 | 1.162 | Duan et al., 1992 |
| Train | 220 | 1640 | 1.221 | Duan et al., 1992 |
| Train | 320 | 1640 | 1.442 | Duan et al., 1992 |
| Train | 345 | 1640 | 1.475 | Duan et al., 1992 |
| Train | 400 | 1640 | 1.527 | Duan et al., 1992 |
| Train | 420 | 1640 | 1.543 | Duan et al., 1992 |
| Train | 450 | 1640 | 1.555 | Duan et al., 1992 |
| Train | 460 | 1640 | 1.559 | Duan et al., 1992 |
| Train | 500 | 1640 | 1.570 | Duan et al., 1992 |
| Train | 545 | 1640 | 1.575 | Duan et al., 1992 |
| Train | 600 | 1640 | 1.574 | Duan et al., 1992 |
| Train | 620 | 1640 | 1.571 | Duan et al., 1992 |
| Train | 800 | 1640 | 1.533 | Duan et al., 1992 |
| Train | 820 | 1640 | 1.528 | Duan et al., 1992 |
| Train | 1000 | 1640 | 1.479 | Duan et al., 1992 |
| Train | 0 | 1680 | 0.271 | Duan et al., 1992 |
| Train | 40 | 1680 | 0.451 | Duan et al., 1992 |
| Train | 60 | 1680 | 0.550 | Duan et al., 1992 |
| Train | 80 | 1680 | 0.658 | Duan et al., 1992 |
| Train | 120 | 1680 | 0.853 | Duan et al., 1992 |
| Train | 200 | 1680 | 1.188 | Duan et al., 1992 |
| Train | 220 | 1680 | 1.250 | Duan et al., 1992 |
| Train | 320 | 1680 | 1.472 | Duan et al., 1992 |
| Train | 345 | 1680 | 1.502 | Duan et al., 1992 |
| Train | 400 | 1680 | 1.554 | Duan et al., 1992 |
| Train | 420 | 1680 | 1.568 | Duan et al., 1992 |
| Train | 450 | 1680 | 1.582 | Duan et al., 1992 |
| Train | 460 | 1680 | 1.585 | Duan et al., 1992 |
| Train | 500 | 1680 | 1.596 | Duan et al., 1992 |
| Train | 545 | 1680 | 1.600 | Duan et al., 1992 |
| Train | 600 | 1680 | 1.597 | Duan et al., 1992 |
| Train | 620 | 1680 | 1.594 | Duan et al., 1992 |
| Train | 800 | 1680 | 1.553 | Duan et al., 1992 |
| Train | 820 | 1680 | 1.547 | Duan et al., 1992 |
| Train | 1000 | 1680 | 1.495 | Duan et al., 1992 |
| Train | 0 | 1720 | 0.281 | Duan et al., 1992 |
| Train | 40 | 1720 | 0.467 | Duan et al., 1992 |
| Train | 60 | 1720 | 0.567 | Duan et al., 1992 |
| Train | 80 | 1720 | 0.676 | Duan et al., 1992 |
| Train | 120 | 1720 | 0.876 | Duan et al., 1992 |
| Train | 200 | 1720 | 1.214 | Duan et al., 1992 |
| Train | 220 | 1720 | 1.279 | Duan et al., 1992 |
| Train | 320 | 1720 | 1.500 | Duan et al., 1992 |
| Train | 345 | 1720 | 1.531 | Duan et al., 1992 |
| Train | 400 | 1720 | 1.583 | Duan et al., 1992 |
| Train | 420 | 1720 | 1.595 | Duan et al., 1992 |
| Train | 450 | 1720 | 1.610 | Duan et al., 1992 |
| Train | 460 | 1720 | 1.612 | Duan et al., 1992 |
| Train | 500 | 1720 | 1.622 | Duan et al., 1992 |
| Train | 545 | 1720 | 1.624 | Duan et al., 1992 |
| Train | 600 | 1720 | 1.620 | Duan et al., 1992 |
| Train | 620 | 1720 | 1.618 | Duan et al., 1992 |
| Train | 800 | 1720 | 1.572 | Duan et al., 1992 |
| Train | 820 | 1720 | 1.566 | Duan et al., 1992 |
| Train | 1000 | 1720 | 1.511 | Duan et al., 1992 |
| Train | 0 | 1760 | 0.291 | Duan et al., 1992 |
| Train | 40 | 1760 | 0.483 | Duan et al., 1992 |
| Train | 60 | 1760 | 0.586 | Duan et al., 1992 |
| Train | 80 | 1760 | 0.696 | Duan et al., 1992 |
| Train | 120 | 1760 | 0.900 | Duan et al., 1992 |
| Train | 200 | 1760 | 1.242 | Duan et al., 1992 |
| Train | 220 | 1760 | 1.310 | Duan et al., 1992 |
| Train | 320 | 1760 | 1.529 | Duan et al., 1992 |
| Train | 345 | 1760 | 1.562 | Duan et al., 1992 |
| Train | 400 | 1760 | 1.612 | Duan et al., 1992 |
| Train | 420 | 1760 | 1.623 | Duan et al., 1992 |
| Train | 450 | 1760 | 1.638 | Duan et al., 1992 |
| Train | 460 | 1760 | 1.640 | Duan et al., 1992 |
| Train | 500 | 1760 | 1.648 | Duan et al., 1992 |
| Train | 545 | 1760 | 1.649 | Duan et al., 1992 |
| Train | 600 | 1760 | 1.644 | Duan et al., 1992 |
| Train | 620 | 1760 | 1.640 | Duan et al., 1992 |
| Train | 800 | 1760 | 1.591 | Duan et al., 1992 |
| Train | 820 | 1760 | 1.585 | Duan et al., 1992 |
| Train | 1000 | 1760 | 1.527 | Duan et al., 1992 |
| Train | 0 | 1800 | 0.303 | Duan et al., 1992 |
| Train | 40 | 1800 | 0.501 | Duan et al., 1992 |
| Train | 60 | 1800 | 0.605 | Duan et al., 1992 |
| Train | 80 | 1800 | 0.716 | Duan et al., 1992 |
| Train | 120 | 1800 | 0.926 | Duan et al., 1992 |
| Train | 200 | 1800 | 1.270 | Duan et al., 1992 |
| Train | 220 | 1800 | 1.342 | Duan et al., 1992 |
| Train | 320 | 1800 | 1.558 | Duan et al., 1992 |
| Train | 345 | 1800 | 1.594 | Duan et al., 1992 |
| Train | 400 | 1800 | 1.643 | Duan et al., 1992 |
| Train | 420 | 1800 | 1.652 | Duan et al., 1992 |
| Train | 450 | 1800 | 1.665 | Duan et al., 1992 |
| Train | 460 | 1800 | 1.669 | Duan et al., 1992 |
| Train | 500 | 1800 | 1.674 | Duan et al., 1992 |
| Train | 545 | 1800 | 1.675 | Duan et al., 1992 |
| Train | 600 | 1800 | 1.669 | Duan et al., 1992 |
| Train | 620 | 1800 | 1.664 | Duan et al., 1992 |
| Train | 800 | 1800 | 1.612 | Duan et al., 1992 |
| Train | 820 | 1800 | 1.605 | Duan et al., 1992 |
| Train | 1000 | 1800 | 1.544 | Duan et al., 1992 |
| Train | 0 | 1840 | 0.314 | Duan et al., 1992 |
| Train | 40 | 1840 | 0.519 | Duan et al., 1992 |
| Train | 60 | 1840 | 0.625 | Duan et al., 1992 |
| Train | 80 | 1840 | 0.738 | Duan et al., 1992 |
| Train | 120 | 1840 | 0.952 | Duan et al., 1992 |
| Train | 200 | 1840 | 1.300 | Duan et al., 1992 |
| Train | 220 | 1840 | 1.371 | Duan et al., 1992 |
| Train | 320 | 1840 | 1.589 | Duan et al., 1992 |
| Train | 345 | 1840 | 1.625 | Duan et al., 1992 |
| Train | 400 | 1840 | 1.671 | Duan et al., 1992 |
| Train | 420 | 1840 | 1.683 | Duan et al., 1992 |
| Train | 450 | 1840 | 1.693 | Duan et al., 1992 |
| Train | 460 | 1840 | 1.696 | Duan et al., 1992 |
| Train | 500 | 1840 | 1.702 | Duan et al., 1992 |
| Train | 545 | 1840 | 1.703 | Duan et al., 1992 |
| Train | 600 | 1840 | 1.694 | Duan et al., 1992 |
| Train | 620 | 1840 | 1.689 | Duan et al., 1992 |
| Train | 800 | 1840 | 1.632 | Duan et al., 1992 |
| Train | 820 | 1840 | 1.625 | Duan et al., 1992 |
| Train | 1000 | 1840 | 1.561 | Duan et al., 1992 |
| Train | 0 | 1880 | 0.327 | Duan et al., 1992 |
| Train | 40 | 1880 | 0.538 | Duan et al., 1992 |
| Train | 60 | 1880 | 0.645 | Duan et al., 1992 |
| Train | 80 | 1880 | 0.760 | Duan et al., 1992 |
| Train | 120 | 1880 | 0.980 | Duan et al., 1992 |
| Train | 200 | 1880 | 1.331 | Duan et al., 1992 |
| Train | 220 | 1880 | 1.401 | Duan et al., 1992 |
| Train | 320 | 1880 | 1.622 | Duan et al., 1992 |
| Train | 345 | 1880 | 1.655 | Duan et al., 1992 |
| Train | 400 | 1880 | 1.701 | Duan et al., 1992 |
| Train | 420 | 1880 | 1.715 | Duan et al., 1992 |
| Train | 450 | 1880 | 1.722 | Duan et al., 1992 |
| Train | 460 | 1880 | 1.725 | Duan et al., 1992 |
| Train | 500 | 1880 | 1.731 | Duan et al., 1992 |
| Train | 545 | 1880 | 1.729 | Duan et al., 1992 |
| Train | 600 | 1880 | 1.719 | Duan et al., 1992 |
| Train | 620 | 1880 | 1.715 | Duan et al., 1992 |
| Train | 800 | 1880 | 1.653 | Duan et al., 1992 |
| Train | 820 | 1880 | 1.646 | Duan et al., 1992 |
| Train | 1000 | 1880 | 1.578 | Duan et al., 1992 |
| Train | 0 | 1920 | 0.340 | Duan et al., 1992 |
| Train | 40 | 1920 | 0.558 | Duan et al., 1992 |
| Train | 60 | 1920 | 0.667 | Duan et al., 1992 |
| Train | 80 | 1920 | 0.783 | Duan et al., 1992 |
| Train | 120 | 1920 | 1.009 | Duan et al., 1992 |
| Train | 200 | 1920 | 1.364 | Duan et al., 1992 |
| Train | 220 | 1920 | 1.433 | Duan et al., 1992 |
| Train | 320 | 1920 | 1.656 | Duan et al., 1992 |
| Train | 345 | 1920 | 1.687 | Duan et al., 1992 |
| Train | 400 | 1920 | 1.732 | Duan et al., 1992 |
| Train | 420 | 1920 | 1.744 | Duan et al., 1992 |
| Train | 450 | 1920 | 1.753 | Duan et al., 1992 |
| Train | 460 | 1920 | 1.755 | Duan et al., 1992 |
| Train | 500 | 1920 | 1.761 | Duan et al., 1992 |
| Train | 545 | 1920 | 1.756 | Duan et al., 1992 |
| Train | 600 | 1920 | 1.744 | Duan et al., 1992 |
| Train | 620 | 1920 | 1.740 | Duan et al., 1992 |
| Train | 800 | 1920 | 1.674 | Duan et al., 1992 |
| Train | 820 | 1920 | 1.666 | Duan et al., 1992 |
| Train | 1000 | 1920 | 1.596 | Duan et al., 1992 |
| Train | 0 | 1960 | 0.354 | Duan et al., 1992 |
| Train | 40 | 1960 | 0.580 | Duan et al., 1992 |
| Train | 60 | 1960 | 0.690 | Duan et al., 1992 |
| Train | 80 | 1960 | 0.808 | Duan et al., 1992 |
| Train | 120 | 1960 | 1.039 | Duan et al., 1992 |
| Train | 200 | 1960 | 1.398 | Duan et al., 1992 |
| Train | 220 | 1960 | 1.466 | Duan et al., 1992 |
| Train | 320 | 1960 | 1.691 | Duan et al., 1992 |
| Train | 345 | 1960 | 1.720 | Duan et al., 1992 |
| Train | 400 | 1960 | 1.765 | Duan et al., 1992 |
| Train | 420 | 1960 | 1.775 | Duan et al., 1992 |
| Train | 450 | 1960 | 1.785 | Duan et al., 1992 |
| Train | 460 | 1960 | 1.786 | Duan et al., 1992 |
| Train | 500 | 1960 | 1.790 | Duan et al., 1992 |
| Train | 545 | 1960 | 1.784 | Duan et al., 1992 |
| Train | 600 | 1960 | 1.771 | Duan et al., 1992 |
| Train | 620 | 1960 | 1.765 | Duan et al., 1992 |
| Train | 800 | 1960 | 1.696 | Duan et al., 1992 |
| Train | 820 | 1960 | 1.687 | Duan et al., 1992 |
| Train | 1000 | 1960 | 1.613 | Duan et al., 1992 |
| Train | 0 | 2000 | 0.368 | Duan et al., 1992 |
| Train | 40 | 2000 | 0.602 | Duan et al., 1992 |
| Train | 60 | 2000 | 0.714 | Duan et al., 1992 |
| Train | 80 | 2000 | 0.833 | Duan et al., 1992 |
| Train | 120 | 2000 | 1.071 | Duan et al., 1992 |
| Train | 200 | 2000 | 1.434 | Duan et al., 1992 |
| Train | 220 | 2000 | 1.501 | Duan et al., 1992 |
| Train | 320 | 2000 | 1.728 | Duan et al., 1992 |
| Train | 345 | 2000 | 1.754 | Duan et al., 1992 |
| Train | 400 | 2000 | 1.799 | Duan et al., 1992 |
| Train | 420 | 2000 | 1.807 | Duan et al., 1992 |
| Train | 450 | 2000 | 1.819 | Duan et al., 1992 |
| Train | 460 | 2000 | 1.818 | Duan et al., 1992 |
| Train | 500 | 2000 | 1.819 | Duan et al., 1992 |
| Train | 545 | 2000 | 1.813 | Duan et al., 1992 |
| Train | 600 | 2000 | 1.799 | Duan et al., 1992 |
| Train | 620 | 2000 | 1.791 | Duan et al., 1992 |
| Train | 800 | 2000 | 1.718 | Duan et al., 1992 |
| Train | 820 | 2000 | 1.709 | Duan et al., 1992 |
| Train | 1000 | 2000 | 1.631 | Duan et al., 1992 |

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