Predicting the temperature and reactant concentration profiles of reacting flow in the partial oxidation of hot coke oven gas using detailed chemistry and a one-dimensional flow model

Supplementary data for the boundary conditions used in the numerical simulations for all the runs.

Run No	1	2	3	4	5	6	7
inlet T, K	625.15	625.15	624.15	623.15	627.15	626.15	626.15
Velocity, m/s@inlet T	0.17439	0.17865	0.16738	0.16333	0.18022	0.18181	0.19243
compounds	mole fraction						
H_2	3.991E-01	3.999E-01	3.976E-01	3.976E-01	3.514E-01	3.559E-01	3.443E-01
CH_4	1.354E-01	1.404E-01	1.434E-01	1.475E-01	1.374E-01	1.318E-01	1.151E-01
C_2H_4	1.028E-02	1.039E-02	1.030E-02	1.037E-02	1.037E-02	9.925E-03	8.476E-03
C_2H_6	4.917E-03	5.025E-03	5.108E-03	5.168E-03	4.965E-03	4.747E-03	3.913E-03
CO	3.327E-02	3.383E-02	3.371E-02	3.374E-02	3.232E-02	3.173E-02	2.949E-02
CO_2	1.202E-02	1.166E-02	1.154E-02	1.135E-02	1.263E-02	1.227E-02	1.089E-02
N_2	1.745E-02	1.966E-02	2.065E-02	2.055E-02	1.362E-02	1.455E-02	1.966E-02
O_2	1.942E-01	1.911E-01	1.972E-01	2.018E-01	1.840E-01	1.881E-01	1.721E-01
H_2O	1.829E-01	1.774E-01	1.698E-01	1.614E-01	2.451E-01	2.428E-01	2.886E-01
benzene	3.262E-03	3.558E-03	3.698E-03	3.916E-03	3.175E-03	3.165E-03	2.947E-03
toluene	6.899E-04	6.988E-04	7.014E-04	7.062E-04	6.927E-04	6.904E-04	6.004E-04
xylene	6.272E-05	6.353E-05	6.377E-05	6.420E-05	5.773E-05	5.754E-05	5.458E-05
styrene	2.031E-04	2.002E-04	1.950E-04	1.841E-04	1.348E-04	1.350E-04	1.221E-04
phenol	4.443E-04	4.379E-04	4.264E-04	4.027E-04	2.948E-04	2.953E-04	2.671E-04
indene	5.840E-04	5.756E-04	5.605E-04	5.293E-04	3.875E-04	3.881E-04	3.511E-04
naphthalene	3.246E-03	3.199E-03	3.115E-03	2.942E-03	2.154E-03	2.157E-03	1.951E-03
2-methylnaphthalene	2.838E-04	2.798E-04	2.724E-04	2.573E-04	1.883E-04	1.886E-04	1.707E-04
1-methylnaphthalene	1.265E-04	1.247E-04	1.214E-04	1.147E-04	8.396E-05	8.410E-05	7.608E-05
acenaphthylene	2.236E-04	2.204E-04	2.147E-04	2.027E-04	1.484E-04	1.486E-04	1.345E-04
acenaphthene	4.572E-05	4.507E-05	4.389E-05	4.144E-05	3.034E-05	3.039E-05	2.749E-05
fluorine	1.404E-04	1.384E-04	1.348E-04	1.273E-04	9.317E-05	9.332E-05	8.443E-05
phenanthrene	4.556E-04	4.491E-04	4.373E-04	4.130E-04	3.023E-04	3.028E-04	2.739E-04
anthracene	1.146E-04	1.129E-04	1.100E-04	1.039E-04	7.603E-05	7.615E-05	6.889E-05
cyclopenta[def]phenanthrene	1.789E-05	1.763E-05	1.717E-05	1.622E-05	1.187E-05	1.189E-05	1.076E-05
2-phenylnaphthalene	8.331E-06	8.212E-06	7.997E-06	7.552E-06	5.528E-06	5.537E-06	5.009E-06
fluoranthene	1.839E-04	1.813E-04	1.765E-04	1.667E-04	1.220E-04	1.222E-04	1.106E-04
acephnanthrylene	7.212E-06	7.109E-06	6.922E-06	6.537E-06	4.785E-06	4.793E-06	4.336E-06
aceanthrylene	6.010E-06	5.924E-06	5.769E-06	5.448E-06	3.988E-06	3.994E-06	3.614E-06
pyrene	1.262E-04	1.244E-04	1.211E-04	1.144E-04	8.374E-05	8.388E-05	7.588E-05
benzo[a]fluorine	1.012E-05	9.972E-06	9.710E-06	9.170E-06	6.713E-06	6.724E-06	6.083E-06
cyclopenta[cd]pyrene	3.223E-06	3.177E-06	3.094E-06	2.921E-06	2.139E-06	2.142E-06	1.938E-06

benz[a]anthracene	5.005E-05	4.933E-05	4.804E-05	4.537E-05	3.321E-05	3.327E-05	3.009E-05
chrysene	5.325E-05	5.248E-05	5.111E-05	4.826E-05	3.533E-05	3.539E-05	3.201E-05
benzo[b]fluoranthene	4.047E-05	3.989E-05	3.884E-05	3.668E-05	2.685E-05	2.690E-05	2.433E-05
benzo[e]pyrene	3.083E-05	3.039E-05	2.959E-05	2.795E-05	2.046E-05	2.049E-05	1.854E-05
benzo[a]pyrene	3.276E-05	3.229E-05	3.144E-05	2.969E-05	2.174E-05	2.177E-05	1.970E-05
perylene	8.671E-06	8.547E-06	8.323E-06	7.860E-06	5.754E-06	5.763E-06	5.214E-06
benzo[ghi]perylene	1.320E-05	1.301E-05	1.267E-05	1.196E-05	8.756E-06	8.770E-06	7.934E-06
anthanthrene	5.278E-06	5.203E-06	5.066E-06	4.784E-06	3.502E-06	3.508E-06	3.174E-06
coronene	1.619E-06	1.596E-06	1.554E-06	1.467E-06	1.074E-06	1.076E-06	9.732E-07

Run No	8	9	10	11	12	13	14
inlet T, K	626.15	642.15	641.15	638.15	637.15	636.15	636.15
Velocity, m/s@inlet T	0.19088	0.23477	0.23054	0.21756	0.23205	0.20553	0.20121
compounds	Mole fraction						
H_2	3.453E-01	4.256E-01	4.194E-01	4.413E-01	3.162E-01	2.664E-01	2.530E-01
CH_4	1.136E-01	1.301E-01	1.373E-01	1.439E-01	1.215E-01	1.568E-01	1.519E-01
C_2H_4	8.044E-03	7.987E-03	8.506E-03	7.261E-03	1.067E-02	1.291E-02	1.189E-02
C_2H_6	3.730E-03	2.667E-03	2.952E-03	2.602E-03	3.830E-03	4.121E-03	3.546E-03
CO	2.931E-02	3.344E-02	3.317E-02	3.374E-02	3.075E-02	3.458E-02	3.591E-02
CO_2	1.062E-02	9.553E-03	1.129E-02	8.276E-03	1.158E-02	1.461E-02	1.476E-02
N_2	2.076E-02	1.418E-02	1.445E-02	2.279E-02	2.077E-02	2.021E-02	3.559E-02
O_2	1.678E-01	1.866E-01	1.915E-01	1.855E-01	1.742E-01	1.957E-01	1.993E-01
H_2O	2.935E-01	1.784E-01	1.710E-01	1.461E-01	2.999E-01	2.832E-01	2.836E-01
benzene	2.945E-03	3.373E-03	3.515E-03	3.362E-03	3.011E-03	4.158E-03	4.181E-03
toluene	5.454E-04	5.091E-04	5.112E-04	4.034E-04	6.339E-04	7.276E-04	6.193E-04
xylene	5.454E-05	6.364E-05	6.391E-05	0.000E+00	5.282E-05	5.197E-05	5.161E-05
styrene	1.213E-04	2.013E-04	1.963E-04	1.468E-04	1.831E-04	1.791E-04	1.777E-04
phenol	2.653E-04	4.404E-04	4.295E-04	3.211E-04	4.006E-04	3.917E-04	3.887E-04
indene	3.488E-04	5.788E-04	5.645E-04	4.221E-04	5.266E-04	5.148E-04	5.110E-04
naphthalene	1.938E-03	3.217E-03	3.137E-03	2.346E-03	2.927E-03	2.861E-03	2.840E-03
2-methylnaphthalene	1.695E-04	2.813E-04	2.744E-04	2.052E-04	2.559E-04	2.502E-04	2.484E-04
1-methylnaphthalene	7.557E-05	1.254E-04	1.223E-04	9.145E-05	1.141E-04	1.116E-04	1.107E-04
acenaphthylene	1.336E-04	2.217E-04	2.162E-04	1.616E-04	2.017E-04	1.972E-04	1.957E-04
acenaphthene	2.731E-05	4.532E-05	4.420E-05	3.305E-05	4.123E-05	4.031E-05	4.001E-05
fluorine	8.386E-05	1.392E-04	1.357E-04	1.015E-04	1.266E-04	1.238E-04	1.229E-04
phenanthrene	2.721E-04	4.516E-04	4.404E-04	3.293E-04	4.108E-04	4.017E-04	3.987E-04

anthracene	6.843E-05	1.136E-04	1.108E-04	8.282E-05	1.033E-04	1.010E-04	1.003E-04
cyclopenta[def]phenanthrene	1.069E-05	1.773E-05	1.729E-05	1.293E-05	1.613E-05	1.577E-05	1.565E-05
2-phenylnaphthalene	4.976E-06	8.258E-06	8.054E-06	6.022E-06	7.513E-06	7.345E-06	7.290E-06
fluoranthene	1.098E-04	1.823E-04	1.778E-04	1.329E-04	1.658E-04	1.621E-04	1.609E-04
acephnanthrylene	4.307E-06	7.149E-06	6.971E-06	5.213E-06	6.503E-06	6.358E-06	6.311E-06
aceanthrylene	3.589E-06	5.957E-06	5.810E-06	4.344E-06	5.419E-06	5.298E-06	5.259E-06
pyrene	7.538E-05	1.251E-04	1.220E-04	9.122E-05	1.138E-04	1.113E-04	1.104E-04
benzo[a]fluorine	6.042E-06	1.003E-05	9.779E-06	7.312E-06	9.122E-06	8.919E-06	8.852E-06
cyclopenta[cd]pyrene	1.925E-06	3.195E-06	3.116E-06	2.330E-06	2.906E-06	2.841E-06	2.820E-06
benz[a]anthracene	2.989E-05	4.961E-05	4.838E-05	3.618E-05	4.513E-05	4.413E-05	4.380E-05
chrysene	3.180E-05	5.278E-05	5.147E-05	3.848E-05	4.801E-05	4.694E-05	4.659E-05
benzo[b]fluoranthene	2.417E-05	4.011E-05	3.912E-05	2.925E-05	3.649E-05	3.568E-05	3.541E-05
benzo[e]pyrene	1.841E-05	3.056E-05	2.980E-05	2.228E-05	2.780E-05	2.718E-05	2.698E-05
benzo[a]pyrene	1.957E-05	3.247E-05	3.167E-05	2.368E-05	2.954E-05	2.888E-05	2.866E-05
perylene	5.179E-06	8.595E-06	8.382E-06	6.268E-06	7.819E-06	7.645E-06	7.588E-06
benzo[ghi]perylene	7.881E-06	1.308E-05	1.276E-05	9.538E-06	1.190E-05	1.163E-05	1.155E-05
anthanthrene	3.152E-06	5.232E-06	5.102E-06	3.815E-06	4.759E-06	4.653E-06	4.619E-06
coronene	9.668E-07	1.604E-06	1.565E-06	1.170E-06	1.460E-06	1.427E-06	1.416E-06

Run No	15	16	17	18	19
inlet T, K	637.15	664.15	653.15	653.15	651.15
Velocity, m/s@inlet T	0.20985	0.21051	0.20735	0.20707	0.21747
compounds	Mole fraction				
H_2	2.701E-01	2.631E-01	3.050E-01	3.146E-01	3.415E-01
CH_4	1.595E-01	1.743E-01	1.697E-01	1.623E-01	1.486E-01
C_2H_4	1.263E-02	1.271E-02	1.055E-02	1.117E-02	9.942E-03
C_2H+6	4.213E-03	4.012E-03	3.263E-03	3.409E-03	3.154E-03
CO	3.480E-02	3.118E-02	3.285E-02	3.303E-02	3.260E-02
CO_2	1.397E-02	1.244E-02	1.214E-02	1.226E-02	1.126E-02
N_2	1.899E-02	9.454E-03	9.367E-03	1.019E-02	9.994E-03
O_2	1.914E-01	2.206E-01	2.135E-01	2.151E-01	2.036E-01
H_2O	2.838E-01	2.550E-01	2.292E-01	2.250E-01	2.255E-01
benzene	4.344E-03	4.846E-03	4.510E-03	4.142E-03	3.764E-03
toluene	5.757E-04	7.295E-04	6.682E-04	5.597E-04	5.704E-04
xylene	5.234E-05	5.211E-05	5.568E-05	5.597E-05	5.704E-05

styrene	1.804E-04	3.243E-04	2.523E-04	2.560E-04	2.636E-04
phenol	3.946E-04	7.094E-04	5.519E-04	5.599E-04	5.766E-04
indene	5.186E-04	9.325E-04	7.254E-04	7.360E-04	7.580E-04
naphthalene	2.882E-03	5.183E-03	4.032E-03	4.090E-03	4.213E-03
2-methylnaphthalene	2.521E-04	4.532E-04	3.526E-04	3.577E-04	3.684E-04
1-methylnaphthalene	1.124E-04	2.020E-04	1.572E-04	1.595E-04	1.642E-04
acenaphthylene	1.986E-04	3.571E-04	2.778E-04	2.818E-04	2.903E-04
acenaphthene	4.061E-05	7.301E-05	5.680E-05	5.762E-05	5.935E-05
fluorine	1.247E-04	2.242E-04	1.744E-04	1.770E-04	1.823E-04
phenanthrene	4.046E-04	7.275E-04	5.659E-04	5.742E-04	5.913E-04
anthracene	1.018E-04	1.830E-04	1.423E-04	1.444E-04	1.487E-04
cyclopenta[def]phenanthrene	1.589E-05	2.857E-05	2.222E-05	2.255E-05	2.322E-05
2-phenylnaphthalene	7.399E-06	1.330E-05	1.035E-05	1.050E-05	1.081E-05
fluoranthene	1.633E-04	2.937E-04	2.284E-04	2.318E-04	2.387E-04
acephnanthrylene	6.405E-06	1.152E-05	8.959E-06	9.089E-06	9.361E-06
aceanthrylene	5.338E-06	9.597E-06	7.466E-06	7.574E-06	7.801E-06
pyrene	1.121E-04	2.015E-04	1.568E-04	1.591E-04	1.638E-04
benzo[a]fluorine	8.985E-06	1.615E-05	1.257E-05	1.275E-05	1.313E-05
cyclopenta[cd]pyrene	2.862E-06	5.147E-06	4.004E-06	4.062E-06	4.183E-06
benz[a]anthracene	4.445E-05	7.992E-05	6.217E-05	6.308E-05	6.496E-05
chrysene	4.729E-05	8.502E-05	6.614E-05	6.710E-05	6.911E-05
benzo[b]fluoranthene	3.594E-05	6.462E-05	5.027E-05	5.100E-05	5.252E-05
benzo[e]pyrene	2.738E-05	4.923E-05	3.830E-05	3.886E-05	4.002E-05
benzo[a]pyrene	2.909E-05	5.231E-05	4.069E-05	4.129E-05	4.252E-05
perylene	7.701E-06	1.385E-05	1.077E-05	1.093E-05	1.126E-05
benzo[ghi]perylene	1.172E-05	2.107E-05	1.639E-05	1.663E-05	1.713E-05
anthanthrene	4.688E-06	8.428E-06	6.557E-06	6.652E-06	6.851E-06
coronene	1.438E-06	2.585E-06	2.011E-06	2.040E-06	2.101E-06

The parity plot shows the comparision between the model predictions and measured temperatures along the axial length of the HCOG reformer. The major difference is observed at the first thermocouple, which

was located at nearer to the reactor inlet, and it shows the maximum difference in all the pilot scale runs. The figure also shows the model predictions were with in the ±10 error. Overall, the predictions are good agreement with the temperature measurements.

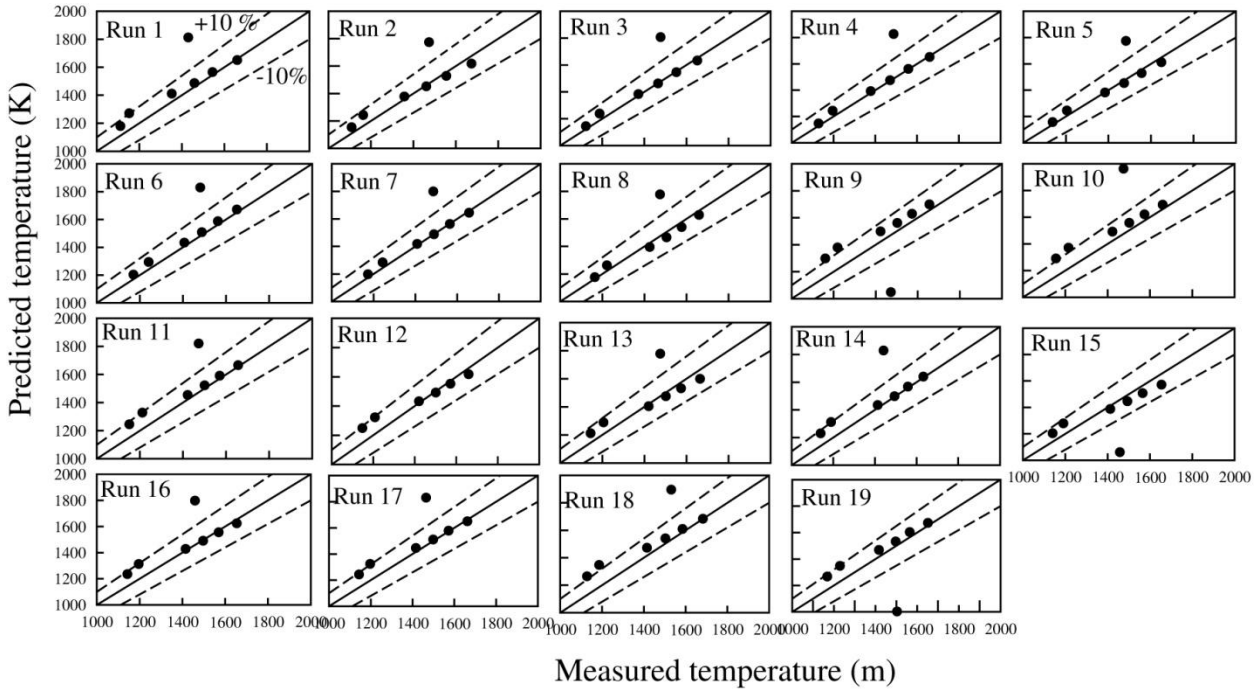

Figure: Comparison between the model predictions and measured temperatures along the axial position of the HCOG reformer. Dashed lines show the ±10 error in the model predictions.

The error analysis was also perfomed for axial diffusion model as provided in the supplementary material, showing that predictions are with ±5% error.

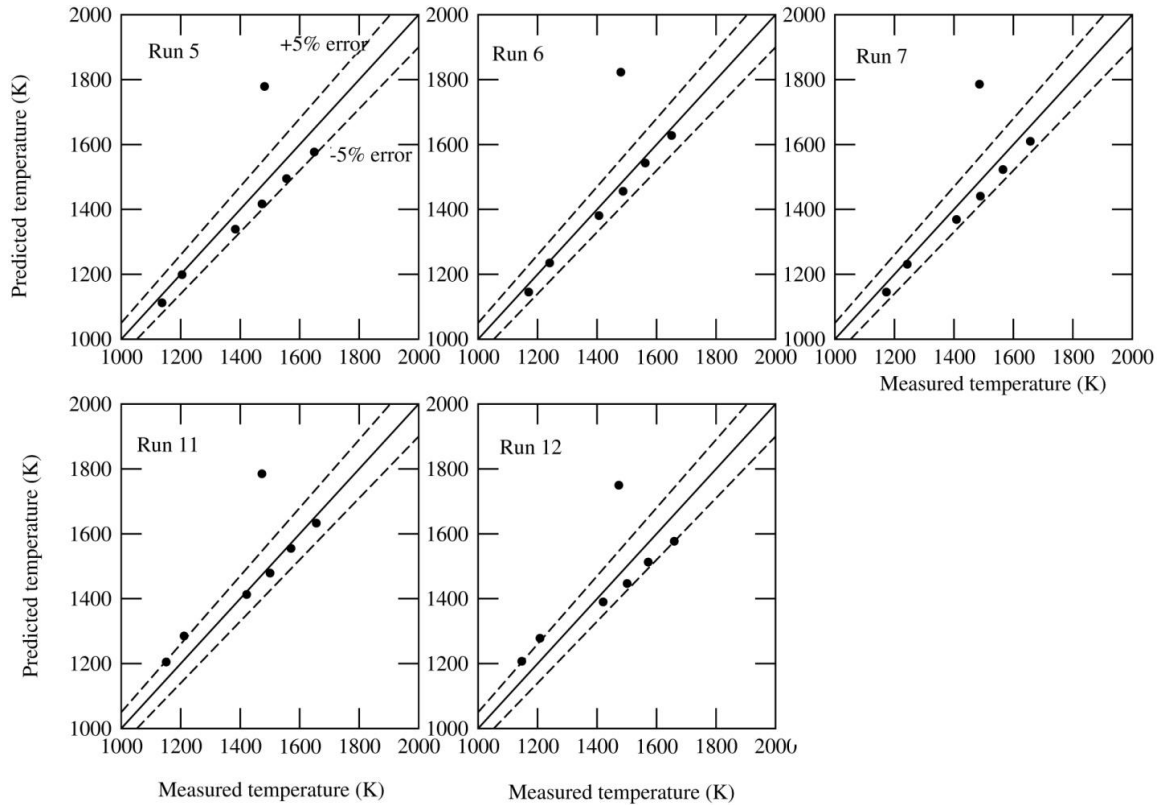

Figure: Comparison between the one dimensional flow with axial diffusion model predictions and measured temperatures along the axial position of the HCOG reformer. Dashed lines show the ±5% error in the model predictions.