Steady state mass balance.

The following were simulated using the following initial concentrations

Cellulose – 0.40

Hemi-Cellulose – 0.3

Lignin – 0.3

Initial Char (if needed) – 10^{-6}

Combustion Model

Detailed Balance (mass fraction)

Compound	600°C	700°C	800°C	900°C
Water Vapor	0.048008	0.053714	0.056133	0.057052
Carbon Monoxide	0.286428	0.340188	0.374004	0.397211
Carbon Dioxide	0.235652	0.210055	0.18662	0.168431
Hydrogen	6.75E-05	0	6.37E-05	0.00019
Methane	0.028089	0.030101	0.031093	0.031569
LVG	0.069885	0.0277	0.012233	0.006149
Phenol	0.006752	0.006552	0.006499	0.006466
Coumaryl	0.015463	0.014856	0.014782	0.014707
HAA	0.090277	0.101524	0.105384	0.107132
Glyoxal	0.014247	0.016542	0.01733	0.017686
Acetaldehyde	0.017218	0.020824	0.022428	0.023138
HMFU	0.029507	0.034317	0.035935	0.03664
Acetone	0.031668	0.036134	0.038038	0.038986
Formic acid	0.004659	0.00519	0.005416	0.005578
Trapped Hydrogen	0.001823	0.001881	0.001848	0.001838
Trapped CO	6.75E-05	0	0	0
Trapped COH_2	0.063065	0.062277	0.062185	0.060983
Xylose	0.010533	0.003698	0.001529	0.000697
Formaldehyde	0.011681	0.013299	0.014017	0.014326
Ethanol	0.007157	0.007266	0.007263	0.007227
Fe_2MaCR	0.027752	0.013883	0.0072	0.003994
Total Mass	**1.481**	**1.5415**	**1.5695**	**1.5775**

Simplified Balance

Compound	600°C	700°C	800°C	900°C
Water Vapor	0.048008	0.053714	0.056133	0.057052
Carbon Monoxide	0.286428	0.340188	0.374004	0.397211
Carbon Dioxide	0.235652	0.210055	0.18662	0.168431
Hydrogen	6.75E-05	0	6.37E-05	0.00019
Methane	0.028089	0.030101	0.031093	0.031569
Phenols	0.049966	0.03529	0.02848	0.025166
Sugars	0.080419	0.031398	0.013762	0.006846
Carbonyls	0.16975	0.193513	0.202612	0.206846
Furans	0.029507	0.034317	0.035935	0.03664
Trapped gases	0.064956	0.064158	0.064033	0.062821
Alcohols	0.007157	0.007266	0.007263	0.007227

Pyrolysis followed by char oxidation.

Detailed Balance (mass fraction)

Compound	600°C	700°C	800°C	900°C
Water Vapor	0.049161	0.053782	0.056278	0.057407
Carbon Monoxide	0.275256	0.34008	0.374442	0.4092
Carbon Dioxide	0.235344	0.210069	0.186552	0.168546
Hydrogen	0	0	6.37E-05	0.001077
Methane	0.028102	0.030103	0.031103	0.031555
LVG	0.073634	0.027702	0.012237	0.006146
Phenol	0.004482	0.006552	0.006501	0.006463
Coumaryl	0.00996	0.014857	0.014786	0.0147
HAA	0.092131	0.101531	0.105481	0.107084
Glyoxal	0.015011	0.016543	0.017336	0.017678
Acetaldehyde	0.018142	0.020825	0.022435	0.023128
HMFU	0.03109	0.034319	0.035946	0.036624
Acetone	0.033367	0.036136	0.03805	0.038968
Formic acid	0.004909	0.00519	0.005417	0.005576
Trapped Hydrogen	0.001921	0.001881	0.001848	0.001774
Trapped CO	0.005051	0	0	0
Trapped COH_2	0.062251	0.062281	0.061504	0.047839
Xylose	0.011098	0.003698	0.00153	0.000697
Formaldehyde	0.012308	0.0133	0.014022	0.01432
Ethanol	0.007541	0.007266	0.007266	0.007223
Fe_2MaCR	0.02924	0.013883	0.007202	0.003992
Total Mass	**1.4056**	**1.5414**	**1.569**	**1.5782**

Simplified Balance

Compound	600°C	700°C	800°C	900°C
Water Vapor	0.049161	0.053782	0.056278	0.057407
Carbon Monoxide	0.275256	0.34008	0.374442	0.4092
Carbon Dioxide	0.235344	0.210069	0.186552	0.168546
Hydrogen	0	0	6.37E-05	0.001077
Methane	0.028102	0.030103	0.031103	0.031555
Phenols	0.043682	0.035293	0.028489	0.025155
Sugars	0.084732	0.0314	0.013767	0.006843
Carbonyls	0.175868	0.193525	0.202741	0.206755
Furans	0.03109	0.034319	0.035946	0.036624
Trapped gases	0.069223	0.064162	0.063352	0.049613
Alcohols	0.007541	0.007266	0.007266	0.007223