**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 | 600oC | 700oC | 800oC | 900oC |
| Time (s) | 100 | 10 | 2 | 1 |
| 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 COH2 | 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 |
| Fe2MaCR | 0.027752 | 0.013883 | 0.0072 | 0.003994 |
| **Total Mass** | **1.481** | **1.5415** | **1.5695** | **1.5775** |

Simplified Balance

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Compound | 600oC | 700oC | 800oC | 900oC |
| Time (s) | 100 | 10 | 2 | 1 |
| 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 | 600oC | 700oC | 800oC | 900oC |
| Time (s) Pyrolysis | 100 | 10 | 2 | 1 |
| Time (s) Oxidation | 0.1 | 0.1 | 0.005 | 0.005 |
| 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 COH2 | 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 |
| Fe2MaCR | 0.02924 | 0.013883 | 0.007202 | 0.003992 |
| **Total Mass** | **1.4056** | **1.5414** | **1.569** | **1.5782** |

Simplified Balance

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Compound | 600oC | 700oC | 800oC | 900oC |
| 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 |