Solution to Assignment 3 2021 Biorefinery

1. Coniferyl alcohol: $C_{10}H_{12}O_3$

a. Synapyl alcohol: $C_{11}H_{14}O_4$

Because they are present as precursors in equimolar amounts in lignin, the elemental formula of lignin is the sum of these two, thus $C_{21}H_{26}O_7$ or $CH_{1.24}O_{0.33}$

b. $HHV = -1.3675 + 0.3137\,C + 0.7009\,H + 0.0318\,O$ with C, H and O as weight percent on dry lignin

$C = 21 \times 12 \times 100/(21\times12 + 26 + 7\times16)$
$= 25200/390 = 64.6\%$
$H = 26\times100/390 = 6.7\%$
$O = 7\times16\times100/390 = 28.7\%$
100.0%

So $HHV_{lignin} = -1.3675 + 0.3137\times64.6 + 0.7009\times6.7 + 0.0318\times28.7\ \frac{MJ}{kg}$

$= 24.5\ MJ/kg$

c. It compares very well with the heating value of 25 MJ/kg in slide 3-43

d. Cellulose: Take 17.4 MJ/kg for HHV from slide 3.43 or calculate: $C_6H_{10}O_5$

$C = 6\times12/(6\times12+10+5\times16)\times100 = 44.4\%$
$H = 10\times100/162 = 6.2\%$
$O = 5\times16\times100/162 = 49.4\%$
100%

So $HHV_{cellulose} = -1.3675 + 0.3137\times44.4 + 0.7009\times6.2 + 0.0318\times49.4 = 18.5\ MJ/kg$

Glucomannan: also $C_6H_{10}O_5$ so value also 18.5 MJ/kg

Xylan: $C_5H_8O_4$ so

$C = 5\times12\times100/(5\times12+8+4\times16) = 6000/132 = 45.4\%$
$H = 8\times100/132 = 6.1\%$
$O = 4\times16\times100/132 = 48.5\%$
100

$HHV_{xylan} = 18.7\ MJ/kg$

Extractives: $C_{10}H_{16}$

$C = 10\times12\times100/(10\times12+16) = 88.2\%$

$H = 16\times100/136 = 11.8\%$

100%

so $HHV = -1.3675 + 0.3137\times88.2 + 0.7009\times11.8 = 35.9$ MJ/kg

Ash: K_2CO_3

$HHV = 0$ MJ/kg

So for Birch

$0.44\times18.5 + 0.28\times18.7 + 0.24\times24.5 + 0.03\times35.9 = 20.3$ MJ/kg

2. a. $\overline{DP_n}$ is $\frac{100}{0.515} - \frac{250}{0.515} = 194 - 485$

This includes the value 400 for MCC.

b. Number of crystalline regions through which one cellulose molecule runs is

$$\frac{10.000}{194\times2} - \frac{10.000}{485\times2} = 26 - 10$$

3. 41% cellulose + 3% glucomannan (all C_6 sugars)

$C_6H_{10}O_5 + H_2O \rightarrow C_6H_{12}O_6$ (glucose)

so per 1 MT of birch: 440 kg $C_6H_{10}O_5$ produces $440\times\frac{180}{162}\times0.9 = 440$ kg C_6 glucose

$C_6H_{12}O_6 \xrightarrow{\text{fermentation}} 2C_2H_5OH + 2CO_2$

so ethanol from C_6: $440\times\frac{2\times46}{180}\times0.95 = 213.6$ kg ethanol

28% xylan (all C_5 sugars)

$C_5H_8O_4 + H_2O \rightarrow C_5H_{10}O_5$ (xylose)

so per 1 MT of birch: $280\times\frac{150}{132}\times0.9 = 286.4$ kg xylose

$6C_5H_{10}O_5 \xrightarrow{\text{fermentation}} 10C_2H_5OH + 10CO_2$

so ethanol from C_5: $286.4\times\frac{10\times46}{6\times150}\times0.80 = 117.1$ kg ethanol

Total ethanol produced: $213.6 + 117.1 = 330.7$ kg ethanol

1 Gallon of ethanol weighs 3.0 kg, so $\frac{330.7}{3} = 110$ Gallon of ethanol