

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 $C_{1.24}H_{1.24}O_{0.33}$

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

$$C = 21 \times 12 \times 100 / (21 \times 12 + 26 + 7 \times 16)$$

$$= 25200 / 390 = 64.6\%$$

$$H = 26 \times 100 / 390 = 6.7\%$$

$$O = 7 \times 16 \times 100 / 390 = 28.7\%$$

$$\text{so } HHV_{\text{lignin}} = -1.3675 + 0.3137 \times 64.6 + 0.7009 \times 6.7 + 0.0318 \times 28.7 \frac{\text{MJ}}{\text{kg}}$$

$$= 24.5 \text{ MJ/kg}$$

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: $C_6H_{10}O_5$

$$C = 6 \times 12 / (6 \times 12 + 10 + 5 \times 16) \times 100 = 44.4\%$$

$$H = 10 \times 100 / 162 = 6.2\%$$

$$O = 5 \times 16 \times 100 / 162 = 49.4\%$$

$$\text{so } HHV_{\text{cellulose}} = -1.3675 + 0.3137 \times 44.4 + 0.7009 \times 6.2 + 0.0318 \times 49.4 = 18.5 \text{ MJ/kg}$$

Glucosmannan: also $C_6H_{10}O_5$ so take also 18.5 MJ/kg

Xylan: $C_5H_8O_4$ so

$$C = 5 \times 12 \times 100 / (5 \times 12 + 8 + 4 \times 16) = 6000 / 132 = 45.4\%$$

$$H = 8 \times 100 / 132 = 6.1\%$$

$$O = 4 \times 16 \times 100 / 132 = 48.5\%$$

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

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

$$C = 10 \times 12 \times 100 / (10 \times 12 + 16) = 88.2\%$$

$$H = 16 \times 100 / 136 = \frac{11.8\%}{100\%}$$

$$\text{So HHV} = -1.3675 + 0.3137 \times 88.2 + 0.7009 \times 11.8 = 35.9 \text{ MJ/kg}$$

Ash: K_2CO_3

$$\text{HHV} = 0 \text{ MJ/kg}$$

so for Birch

$$0.44 \times 18.5 + 0.28 \times 18.7 + 0.24 \times 24.5 + 0.03 \times 35.9 = 20.3 \frac{\text{MJ}}{\text{kg}}$$

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

This includes the value 400 for MCC.

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

$$\frac{10,000}{194 \times 2} - \frac{10,000}{485 \times 2} = 26 - 10$$

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

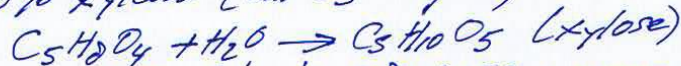


so per 1 MT of birch: 440 kg $C_6H_{10}O_5$ produces $440 \times \frac{180}{162} \times 0.9 = 440 \text{ kg}$ $C_6H_{12}O_6$



so ethanol from C_6 : $440 \times \frac{2 \times 46}{180} \times 0.95 = 213.6 \text{ kg ethanol}$

28% xylan (all C_5 sugars)



so per 1 MT of birch: $280 \times \frac{150}{132} \times 0.9 = 286.4 \text{ kg xylose}$



so ethanol from C_5 : $286.4 \times \frac{10 \times 46}{6 \times 150} \times 0.80 = 117.1 \text{ kg ethanol}$

Total ethanol produced: $213.6 + 117.1 = 330.7 \text{ kg ethanol}$

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