$$[Fuel]C_\alpha H_\beta O_\gamma + 0.79[Air]N_2 + 0.21[Air]O_2 \rightarrow$$
$$[CO2]CO_2 + [CO]CO + [THC]C_{C_f}H_{2C_f+2} + [NO_X]NO + [H_2O]H_2O + [O_2]O_2 + [H_2]H_2 + [N_2]N_2$$

Carbon balance

$$\alpha[Fuel] = [CO_2] + [CO] + C_f[THC]$$

Oxygen balance

$$\gamma[Fuel] + 2 \times 0.21[Air] = 2[CO_2] + [CO] + [NO_X] + [H_2O] + 2[O_2]$$

Hydrogen balance

$$\beta[Fuel] = \left(2C_f + 2\right)[THC] + 2[H_2O] + 2[H_2]$$

CO/CO_2 equilibrium

$$CO_2 + H_2 \leftrightarrows CO + H_2O$$

$$K_{eq} = \frac{[CO][H_2O]}{[CO_2][H_2]} = 3.5\ for\ 1750K\ (mean\ burning\ temperature)$$

Developing equations

Molecular Hydrogen concentration

$$[H_2] = \frac{\beta}{2}[Fuel] - [H_2O] - \left(C_f + 1\right)[THC]$$

Water concentration

$$[H_2O] = K_{eq}\frac{[CO_2]}{[CO]}[H_2] = K_{eq}\frac{[CO_2]}{[CO]}\left\{\frac{\beta}{2}[Fuel] - [H_2O] - \left(C_f + 1\right)[THC]\right\}$$

[THC] is a small term, *O(10^{-5})*,

$$[H_2O] = \frac{\frac{\beta}{2}[Fuel]}{\left\{1 + \frac{[CO]}{K_{eq}[CO_2]}\right\}} = \frac{K_{eq}\frac{\beta}{2}[Fuel]}{\left\{K_{eq} + \frac{[CO]}{[CO_2]}\right\}} = \frac{3.5\frac{\beta}{2}[Fuel]}{\left\{3.5 + \frac{[CO]}{[CO_2]}\right\}}$$

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Fuel concentration

$$[Fuel] = \frac{[CO_2] + [CO] + C_f[THC]}{\alpha}$$

Air concentration

$$0.21[Air] = \frac{1}{2} \times \{2[CO_2] + [CO] + [NO_X] + [H_2O] + 2[O_2]\} - \frac{\gamma}{2}[Fuel]$$

$$0.21[Air] = [CO_2] + \frac{[CO]}{2} + \frac{[NO_X]}{2} + \frac{1}{2} \times \frac{3.5\frac{\beta}{2}[Fuel]}{\left\{3.5 + \frac{[CO]}{[CO_2]}\right\}} + [O_2] - \frac{\gamma}{2}[Fuel]$$

$$0.21[Air] = [CO_2] + \frac{[CO]}{2} + [O_2] + \frac{[NO_X]}{2} + \frac{3.5}{\left\{3.5 + \frac{[CO]}{[CO_2]}\right\}} \times \frac{\beta}{4}[Fuel] - \frac{\gamma}{2}[Fuel]$$

$$0.21[Air] = [CO_2] + \frac{[CO]}{2} + [O_2] + \frac{[NO_X]}{2} + \left\{\frac{3.5}{\left\{3.5 + \frac{[CO]}{[CO_2]}\right\}} \times \frac{\beta}{4} - \frac{\gamma}{2}\right\}[Fuel]$$

$$0.21[Air] = [CO_2] + \frac{[CO]}{2} + [O_2] + \frac{[NO_X]}{2} + \left\{\frac{3.5}{\left\{3.5 + \frac{[CO]}{[CO_2]}\right\}} \times \frac{\beta}{4} - \frac{\gamma}{2}\right\}\frac{[CO_2] + [CO] + C_f[THC]}{\alpha}$$

Defining,

$$O_{cv} = \frac{\gamma}{\alpha}$$

$$H_{cv} = \frac{\beta}{\alpha}$$

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$$0.21[Air] = [CO_2] + \frac{[CO]}{2} + [O_2] + \frac{[NO_X]}{2} + \left\{\frac{3.5}{\left\{3.5 + \frac{[CO]}{[CO_2]}\right\}} \times \frac{H_{cv}}{4} - \frac{O_{cv}}{2}\right\}\{[CO_2] + [CO] + C_f[THC]\}$$

[THC] is a small term, *O(10^-5^)*,

$$[Air] = \frac{1}{0.21}\left\{[CO_2] + \frac{[CO]}{2} + [O_2] + \frac{[NO_X]}{2} + \left\{\frac{3.5}{\left\{3.5 + \frac{[CO]}{[CO_2]}\right\}} \times \frac{H_{cv}}{4} - \frac{O_{cv}}{2}\right\}\{[CO_2] + [CO]\}\right\}$$

Air/Fuel ratio calculation (molar base)

$$\frac{[Air]}{[Fuel]} = \frac{\frac{\alpha}{0.21}\left\{[CO_2] + \frac{[CO]}{2} + [O_2] + \frac{[NO_X]}{2} + \left\{\frac{3.5}{\left\{3.5 + \frac{[CO]}{[CO_2]}\right\}} \times \frac{H_{cv}}{4} - \frac{O_{cv}}{2}\right\}\{[CO_2] + [CO]\}\right\}}{\{[CO_2] + [CO] + C_f[THC]\}}$$

For stoichiometric conditions (molar base),

$$[CO] = [O_2] = [NO_x] = [THC] = 0$$

$$\left.\frac{[Air]}{[Fuel]}\right|_{stoich} = \frac{\alpha}{0.21}\left(1 + \frac{H_{cv}}{4} - \frac{O_{cv}}{2}\right)$$

Air/Fuel ratio in mass base,

$$M_{air} = 28.84\frac{kg}{kmol}$$

$$M_{fuel} = 12\alpha + \beta + 16\gamma \quad kg/kmol$$

$$AF = \frac{m_{air}}{m_{fuel}} = \frac{[Air]}{[Fuel]}\frac{M_{air}}{M_{fuel}}$$

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Brettschneider Equation, 1979, for Lambda factor:

$$\lambda = \frac{\frac{[Air]}{[Fuel]}\frac{M_{air}}{M_{fuel}}}{\left.\frac{[Air]}{[Fuel]}\right|_{stoich}\frac{M_{air}}{M_{fuel}}} = \frac{\frac{[Air]}{[Fuel]}}{\left.\frac{[Air]}{[Fuel]}\right|_{stoich}}$$

$$\lambda = \frac{\left\{[CO_2] + \frac{[CO]}{2} + [O_2] + \frac{[NO_X]}{2} + \left\{\frac{3.5}{\left\{3.5 + \frac{[CO]}{[CO_2]}\right\}} \times \frac{H_{cv}}{4} - \frac{O_{cv}}{2}\right\}\{[CO_2] + [CO]\}\right\}}{\left(1 + \frac{H_{cv}}{4} - \frac{O_{cv}}{2}\right)\{[CO_2] + [CO] + C_f[THC]\}}$$

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