

$$\tilde{W} = \frac{12.0107 \left[\frac{3.922 \cdot 0.091634}{1 + 0.02721} + \frac{\tilde{n}_2 \cdot x_{\text{Ccombdry}2}}{1 + x_{\text{H}_2\text{Oexh}2}} + \dots + \frac{\tilde{n}_{3000} \cdot x_{\text{Ccombdry}3000}}{1 + x_{\text{H}_2\text{Oexh}3000}} \right] \cdot 0.2}{285 \cdot 0.869}$$

$\tilde{W} = 5.09 \text{ (kW}\cdot\text{hr)}$

(g) *Rounding.* Round emission values only after all calculations are complete and the result is in g/(kW·hr) or units equivalent to the units of the standard, such as g/(hp·hr). See the definition of "Round" in §1065.1001.

§ 1065.655 Chemical balances of fuel, intake air, and exhaust.

(a) *General.* Chemical balances of fuel, intake air, and exhaust may be used to calculate flows, the amount of water in their flows, and the wet concentration of constituents in their flows. With one flow rate of either fuel, intake air, or exhaust, you may use chemical balances to determine the flows of the other two. For example, you may use chemical balances along with either intake air or fuel flow to determine raw exhaust flow.

(b) *Procedures that require chemical balances.* We require chemical balances when you determine the following:

(1) A value proportional to total work, \tilde{W} , when you choose to determine brake-specific emissions as described in §1065.650(e).

(2) The amount of water in a raw or diluted exhaust flow, $x_{\text{H}_2\text{O}}$, when you do not measure the amount of water to correct for the amount of water removed by a sampling system. Correct for removed water according to §1065.659(c)(2).

(3) The flow-weighted mean fraction of dilution air in diluted exhaust \tilde{x}_{dil} , when you do not measure dilution air flow to correct for background emissions as described in §1065.667(c). Note that if you use chemical balances for this purpose, you are assuming that your exhaust is stoichiometric, even if it is not.

(c) *Chemical balance procedure.* The calculations for a chemical balance involve a system of equations that require iteration. We recommend using a computer to solve this system of equations. You must guess the initial values of up to three quantities: the

amount of water in the measured flow, $x_{\text{H}_2\text{O}}$, fraction of dilution air in diluted exhaust, \tilde{x}_{dil} , and the amount of products on a C_1 basis per dry mole of dry measured flow, x_{Cproddry} . For each emission concentration, x , and amount of water $x_{\text{H}_2\text{O}}$, you must determine their completely dry concentrations, x_{dry} and $x_{\text{H}_2\text{Odry}}$. You must also use your fuel's atomic hydrogen-to-carbon ratio, α , and oxygen-to-carbon ratio, β . For your fuel, you may measure α and β or you may use the default values in Table 1 of §1065.650. Use the following steps to complete a chemical balance:

(1) Convert your measured concentrations such as, $x_{\text{CO}_2\text{meas}}$, x_{NOmeas} , and $x_{\text{H}_2\text{Oint}}$, to dry concentrations by dividing them by one minus the amount of water present during their respective measurements; for example: $x_{\text{H}_2\text{O}x\text{CO}_2}$, $x_{\text{H}_2\text{O}x\text{NO}}$, and $x_{\text{H}_2\text{Oint}}$. If the amount of water present during a "wet" measurement is the same as the unknown amount of water in the exhaust flow, $x_{\text{H}_2\text{O}}$, iteratively solve for that value in the system of equations. If you measure only total NO_x and not NO and NO_2 separately, use good engineering judgement to estimate a split in your total NO_x concentration between NO and NO_2 for the chemical balances. For example, if you measure emissions from a stoichiometric spark-ignition engine, you may assume all NO_x is NO. For a compression-ignition engine, you may assume that your molar concentration of NO_x , x_{NO_x} , is 75% NO and 25% NO_2 . For NO_2 storage aftertreatment systems, you may assume x_{NO_x} is 25% NO and 75% NO_2 . Note that for calculating the mass of NO_x emissions, you must use the molar mass of NO_2 for the effective molar mass of all NO_x species, regardless of the actual NO_2 fraction of NO_x .

(2) Enter the equations in paragraph (c)(4) of this section into a computer program to iteratively solve for $x_{\text{H}_2\text{O}}$ and x_{Cproddry} . If you measure raw exhaust flow, set \tilde{x}_{dil} equal to zero. If you

measure diluted exhaust flow, iteratively solve for x_{dil} . Use good engineering judgment to guess initial values for x_{H_2O} , $x_{C_{proddry}}$, and x_{dil} . We recommend guessing an initial amount of water that is about twice the amount of water in your intake or dilution air. We recommend guessing an initial value of $x_{C_{proddry}}$ as the sum of your measured CO_2 , CO , and THC values. If you measure diluted exhaust, we also recommend guessing an initial x_{dil} between 0.75 and 0.95, such as 0.8. Iterate values in the system of equations until the most recently updated guesses are all within $\pm 1\%$ of their respective most recently calculated values.

(3) Use the following symbols and subscripts in the equations for this paragraph (c):

- x_{H_2O} = Amount of water in measured flow.
- x_{H_2Odry} = Amount of water per dry mole of measured flow.
- $x_{C_{proddry}}$ = Amount of carbon products on a C_1 basis per dry mole of measured flow.
- x_{dil} = Fraction of dilution air in measured flow, assuming stoichiometric exhaust; or x_{dil} = excess air for raw exhaust.

- $x_{prod/intdry}$ = Amount of dry stoichiometric products per dry mole of intake air.
- $x_{O_2proddry}$ = Amount of oxygen products on an O_2 basis per dry mole of measured flow.
- $x_{[emission]dry}$ = Amount of emission per dry mole of measured flow.
- $x_{[emission]meas}$ = Amount of emission in measured flow.
- $x_{H_2O[emission]meas}$ = Amount of water at emission-detection location. Measure or estimate these values according to § 1065.145(d)(2).
- x_{H_2Oint} = Amount of water in the intake air, based on a humidity measurement of intake air.
- x_{H_2Odil} = Amount of water in dilution air, based on a humidity measurement of intake air.
- $x_{O_2airdry}$ = Amount of oxygen per dry mole of air. Use $x_{O_2airdry} = 0.209445$ mol/mol.
- $x_{CO_2airdry}$ = Amount of carbon dioxide per dry mole of air. Use $x_{CO_2airdry} = 375$ μ mol/mol.
- α = Atomic hydrogen-to-carbon ratio in fuel.
- β = Atomic oxygen-to-carbon ratio in fuel.

(4) Use the following equations to iteratively solve for x_{H_2O} and $x_{C_{proddry}}$:

$$x_{H_2O} = \frac{x_{H_2Odry}}{1 + x_{H_2Odry}} \quad \text{Eq. 1065.655-1}$$

$$x_{H_2Odry} = \frac{\alpha}{2} \cdot x_{C_{proddry}} + (1 - x_{dil}) \cdot \frac{x_{H_2Ointdry}}{x_{prod/intdry}} + x_{dil} \cdot x_{H_2Odildry} \quad \text{Eq. 1065.655-2}$$

$$x_{C_{proddry}} = x_{CO_2dry} + x_{COdry} + x_{THCdry} \quad \text{Eq. 1065.655-3}$$

$$x_{dil} = 1 - \frac{x_{O_2proddry} \cdot x_{prod/intdry}}{x_{O_2airdry}} \cdot (1 + x_{H_2Ointdry}) \quad \text{Eq. 1065.655-4}$$

$$x_{prod/intdry} = \frac{1}{1 - \frac{1}{1 - x_{dil}} \cdot \frac{1}{2} \cdot \left(x_{COdry} - \frac{\alpha}{2} \cdot x_{C_{proddry}} - x_{NO_2dry} \right)} \quad \text{Eq. 1065.655-5}$$

$$x_{O_2proddry} = x_{CO_2dry} + \frac{1}{2} \cdot \left(x_{COdry} + \frac{\alpha}{2} \cdot x_{C_{proddry}} + x_{NO_2dry} \right) + x_{NO_2dry} - \beta \cdot x_{C_{proddry}} \quad \text{Eq. 1065.655-6}$$

$$x_{CO_2dry} = \frac{x_{CO_2meas}}{1 - x_{H_2OCO_2meas}} - \frac{x_{CO_2airdry}}{1 - \frac{1}{2} \cdot \left(x_{COdry} - \frac{\alpha}{2} \cdot x_{C_{proddry}} - x_{NO_2dry} \right)} \quad \text{Eq. 1065.655-7}$$

$$x_{COdry} = \frac{x_{COmeas}}{1 - x_{H_2OxCOmeas}} \quad \text{Eq. 1065.655-8}$$

$$x_{THCdry} = \frac{x_{THCmeas}}{1 - x_{H_2OxTHCmeas}} \quad \text{Eq. 1065.655-9}$$

$$x_{\text{H}_2\text{Ointdry}} = \frac{x_{\text{H}_2\text{Oint}}}{1 - x_{\text{H}_2\text{Oint}}} \quad \text{Eq. 1065.655-10}$$

$$x_{\text{H}_2\text{Odildry}} = \frac{x_{\text{H}_2\text{Odil}}}{1 - x_{\text{H}_2\text{Odil}}} \quad \text{Eq. 1065.655-11}$$

$$x_{\text{NO}_2\text{dry}} = \frac{x_{\text{NO}_2\text{meas}}}{1 - x_{\text{H}_2\text{O}} \cdot x_{\text{NO}_2\text{meas}}} \quad \text{Eq. 1065.655-12}$$

$$x_{\text{NOdry}} = \frac{x_{\text{NOmeas}}}{1 - x_{\text{H}_2\text{O}} \cdot x_{\text{NOmeas}}} \quad \text{Eq. 1065.655-13}$$

(5) The following example is a solution for $x_{\text{H}_2\text{O}}$ and $x_{\text{C}_{\text{proddry}}}$ using the equations in paragraph (c)(4) of this section:

$$x_{\text{H}_2\text{O}} = \frac{35.24}{1 + \frac{35.24}{1000}} = 34.04 \text{ mmol/mol}$$

$$x_{\text{H}_2\text{Odry}} = \frac{1.8}{2} \cdot 24.69 + (1 - 0.843) \cdot \frac{17.22}{0.9338} + 0.843 \cdot 12.01 = 35.24 \text{ mmol/mol}$$

$$x_{\text{C}_{\text{proddry}}} = 24.614 + \frac{29.3}{1000} + \frac{47.6}{1000} = 24.69 \text{ mmol/mol}$$

$$x_{\text{dil}} = 1 - \frac{\frac{34.54}{1000} \cdot 0.9338}{0.209445} \cdot \left(1 + \frac{17.22}{1000}\right) = 0.843$$

$$x_{\text{prod/intdry}} = \frac{1}{1 - \frac{1}{1 - 0.843} \cdot \frac{1}{2} \cdot \left(\frac{29.3}{1000000} - \frac{1.8}{2} \cdot \frac{24.69}{1000} - \frac{12.1}{1000000}\right)} = 0.9338 \text{ mol/mol}$$

$$x_{\text{O}_2\text{prod/intdry}} = 24.614 + \frac{1}{2} \cdot \left(\frac{29.3}{1000} + \frac{1.8}{2} \cdot 24.69 + \frac{50.4}{1000}\right) + \frac{12.1}{1000} - 0.05 \cdot 24.69 = 34.54 \text{ mol/mol}$$

$$x_{\text{CO}_2\text{dry}} = \frac{24.770}{1 - \frac{8.601}{1000}} - \frac{\frac{375}{1000}}{1 - \frac{1}{2} \cdot \left(\frac{29.3}{1000000} - \frac{1.8}{2} \cdot \frac{24.69}{1000} - \frac{12.1}{1000000}\right)} = 24.614 \text{ mmol/mol}$$

$\alpha_{\text{gasoline}} = 1.85$	$\beta_{\text{gasoline}} = 0.016$	$W_{\text{C,gasoline}} = 0.866$
$\alpha_{\text{\#2 Diesel}} = 1.80$	$\beta_{\text{\#2 Diesel}} = 0.016$	$W_{\text{C,\#2 Diesel}} = 0.869$
$\alpha_{\text{\#1 Diesel}} = 1.93$	$\beta_{\text{\#1 Diesel}} = 0.016$	$W_{\text{C,\#1 Diesel}} = 0.861$
$\alpha_{\text{LPG}} = 2.64$	$\beta_{\text{LPG}} = 0.016$	$W_{\text{C,LPG}} = 0.819$
$\alpha_{\text{Natural Gas}} = 3.78$	$\beta_{\text{Natural Gas}} = 0.016$	$W_{\text{C,Natural Gas}} = 0.747$
$\alpha_{\text{Ethanol}} = 0.5$	$\beta_{\text{Ethanol}} = 0.016$	$W_{\text{C,Ethanol}} = 0.521$
$\alpha_{\text{Methanol}} = 1$	$\beta_{\text{Methanol}} = 0.016$	$W_{\text{C,Methanol}} = 0.375$

TABLE 1 OF § 1065.655—DEFAULT VALUES OF ATOMIC HYDROGEN-TO-CARBON RATIO, α , ATOMIC OXYGEN-TO-CARBON RATIO, β AND CARBON MASS FRACTION OF FUEL, W_C , FOR VARIOUS FUELS

Fuel	Atomic hydrogen and oxygen-to-carbon ratios $CH_{\alpha}O_{\beta}$	Carbon mass concentration, W_C/g
Gasoline	$CH_{1.85}O_0$	0.866
#2 Diesel	$CH_{1.80}O_0$	0.869
#1 Diesel	$CH_{1.93}O_0$	0.861
Liquified Petroleum Gas	$CH_{2.64}O_0$	0.819
Natural gas	$CH_{3.78}O_{0.016}$	0.747
Ethanol	$CH_0.5O_{0.5}$	0.521
Methanol	CH_1O_1	0.375

(d) *Calculated raw exhaust molar flow rate from measured intake air molar flow rate or fuel mass flow rate.* You may calculate the raw exhaust molar flow rate from which you sampled emissions, \dot{n}_{exh} , based on the measured intake air molar flow rate, \dot{n}_{int} , or the measured fuel mass flow rate, \dot{m}_{fuel} , and the values calculated using the chemical balance in paragraph (c) of this section. Solve for the chemical balance in paragraph (c) of this section at the same frequency that you update and record \dot{n}_{int} or \dot{m}_{fuel} .

(1) *Crankcase flow rate.* You may calculate raw exhaust flow based on \dot{n}_{int} or \dot{m}_{fuel} only if at least one of the following is true about your crankcase emission flow rate:

(i) Your test engine has a production emission-control system with a closed

crankcase that routes crankcase flow back to the intake air, downstream of your intake air flow meter.

(ii) During emission testing you route open crankcase flow to the exhaust according to §1065.130(g).

(iii) You measure open crankcase emissions and flow, and you add the masses of crankcase emissions to your brake-specific emission calculations.

(iv) Using emission data or an engineering analysis, you can show that neglecting the flow rate of open crankcase emissions does not adversely affect your ability to demonstrate compliance with the applicable standards.

(2) *Intake air molar flow rate calculation.* Based on \dot{n}_{int} , calculate \dot{n}_{exh} as follows:

$$\dot{n}_{\text{exh}} = \left[\dot{n}_{\text{int}} \cdot (1 - x_{\text{H2O int}}) \cdot x_{\text{prod/intdry}} \cdot (1 + x_{\text{H2Odry}}) \right] \cdot \left[1 + \frac{x_{\text{dil}}}{1 - x_{\text{dil}}} \right] \quad \text{Eq. 1065.655-14}$$

Where:

\dot{n}_{exh} = raw exhaust molar flow rate from which you measured emissions.

\dot{n}_{int} = intake air molar flow rate including humidity in intake air.

Example:

$\dot{n}_{\text{int}} = 3.780 \text{ mol/s}$

$x_{\text{H2Oint}} = 16.930 \text{ mmol/mol} = 0.016930 \text{ mol/mol}$

$x_{\text{prod/intdry}} = 0.93382 \text{ mol/mol}$

$x_{\text{H2Odry}} = 130.16 \text{ mmol/mol} = 0.13016 \text{ mol/mol}$

$x_{\text{dil}} = 0.20278 \text{ mol/mol}$

$$\dot{n}_{\text{exh}} = [3.780 \cdot (1 - 0.016930) \cdot 0.93382 \cdot (1 + 0.13016)] \cdot \left[1 + \frac{0.20278}{1 - 0.20278} \right]$$

$\dot{n}_{\text{exh}} = 4.919 \text{ mol/s}$

(3) *Fuel mass flow rate calculation.* Based on \dot{m}_{fuel} , calculate \dot{n}_{exh} as follows:

$$\dot{n}_{\text{exh}} = \frac{\dot{m}_{\text{fuel}} \cdot w_c}{M_c \cdot X_{\text{Cproddry}}} \cdot (1 + X_{\text{H2Odry}}) \cdot \left[1 + \frac{X_{\text{dil}}}{1 - X_{\text{dil}}} \right] \quad \text{Eq. 1065.655-15}$$

Where:

\dot{n}_{exh} = raw exhaust molar flow rate from which you measured emissions.

\dot{m}_{fuel} = intake air molar flow rate including humidity in intake air.

Example:

$\dot{m}_{\text{fuel}} = 6.023 \text{ g/s}$

$w_c = 0.869 \text{ g/g}$

$M_c = 12.0107 \text{ g/mol}$

$X_{\text{Cproddry}} = 125.58 \text{ mmol/mol} = 0.12558 \text{ mol/mol}$

$X_{\text{H2Odry}} = 130.16 \text{ mmol/mol} = 0.13016 \text{ mol/mol}$

$X_{\text{dil}} = 0.20278 \text{ mol/mol}$

$$\dot{n}_{\text{exh}} = \frac{6.0233 \cdot 0.869}{12.0107 \cdot 0.12558} \cdot (1 + 0.13016) \cdot \left[1 + \frac{0.20278}{1 - 0.20278} \right]$$

$\dot{n}_{\text{exh}} = 4.919 \text{ mol/s}$

EFFECTIVE DATE NOTE: At 73 FR 37331, June 30, 2008, § 1065.655 was revised, effective July 7, 2008. For the convenience of the user, the revised text is set forth as follows:

§ 1065.655 Chemical balances of fuel, intake air, and exhaust.

(a) *General.* Chemical balances of fuel, intake air, and exhaust may be used to calculate flows, the amount of water in their flows, and the wet concentration of constituents in their flows. With one flow rate of either fuel, intake air, or exhaust, you may use chemical balances to determine the flows of the other two. For example, you may use chemical balances along with either intake air or fuel flow to determine raw exhaust flow.

(b) *Procedures that require chemical balances.* We require chemical balances when you determine the following:

(1) A value proportional to total work, \dot{W} , when you choose to determine brake-specific emissions as described in § 1065.650(e).

(2) The amount of water in a raw or diluted exhaust flow, X_{H2Oexh} , when you do not measure the amount of water to correct for the amount of water removed by a sampling system. Correct for removed water according to § 1065.659(c)(2).

(3) The flow-weighted mean fraction of dilution air in diluted exhaust, $X_{\text{dil/exh}}$, when you do not measure dilution air flow to correct for background emissions as described in § 1065.667(c). Note that if you use chemical balances for this purpose, you are assuming that your exhaust is stoichiometric, even if it is not.

(c) *Chemical balance procedure.* The calculations for a chemical balance involve a system of equations that require iteration. We recommend using a computer to solve this system of equations. You must guess the initial values of up to three quantities: The amount of water in the measured flow, X_{H2Oexh} , fraction of dilution air in diluted exhaust, $X_{\text{dil/exh}}$, and the amount of products on a C_1 basis per dry mole of dry measured flow, X_{Ccombdry} . You may use time-weighted mean values of combustion air humidity and dilution air humidity in the chemical balance; as long as your combustion air and dilution air humidities remain within tolerances of $\pm 0.0025 \text{ mol/mol}$ of their respective mean values over the test interval. For each emission concentration, x , and amount of water, X_{H2Oexh} , you must determine their completely dry concentrations, X_{dry} and $X_{\text{H2Oexhdry}}$. You must also use your fuel's atomic hydrogen-to-carbon ratio, α , and oxygen-to-carbon