40 C.F.R. § 1065.655

Chemical balances of fuel, DEF, 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. Note that chemical balance calculations allow measured values for the flow rate of diesel exhaust fluid for engines with urea-based selective catalytic reduction.

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

(1) A value proportional to total work, *Wñ*, when you choose to determine brake-specific emissions as described in § 1065.650(f).

(2) Raw exhaust molar flow rate either from measured intake air molar flow rate or from fuel mass flow rate as described in paragraph (f) of this section.

(3) Raw exhaust molar flow rate from measured intake air molar flow rate and dilute exhaust molar flow rate, as described in paragraph (g) of this section.

(4) The amount of water in a raw or diluted exhaust flow, χ_{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.

(5) The calculated total dilution air flow when you do not measure dilution air flow to correct for background emissions as described in § 1065.667(c) and (d).

(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, $x_{dil/exh}$, 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 intake air humidity and dilution air humidity in the chemical balance; as long as your intake air and dilution air humidities remain within tolerances of ±0.0025 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 $x_{H2Oexhdry}$. You must also use your fuel mixture's atomic hydrogen-to-carbon ratio, α, oxygen-to-carbon ratio, β, sulfur-to-carbon ratio, γ, and nitrogen-to-carbon ratio, δ; you may optionally account for diesel exhaust fluid (or other fluids injected into the exhaust), if applicable. You may calculate α, β, γ, and δ based on measured fuel composition or based on measured fuel and diesel exhaust fluid (or other fluids injected into the exhaust) composition together, as described in paragraph (e) of this section. You may alternatively use any combination of default values and measured values as described in paragraph (e) of this section. Use the following steps to complete a chemical balance:

(1) Convert your measured concentrations such as, $x_{CO2meas}$, x_{NOmeas}, and x_{H2Oint}, to dry concentrations by dividing them by one minus the amount of water present during their respective measurements; for example: $x_{H2OxCO2meas}$, $x_{H2OxNOmeas}$, and x_{H2Oint}. If the amount of water present during a "wet" measurement is the same as the unknown amount of water in the exhaust flow, x_{H2Oexh}, 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 judgment 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_{NOx}, is 75% NO and 25% NO_2. For NO_2 storage aftertreatment systems, you may assume x_{NOx} 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.