Appendix E

Stoichiometric Flow Control Calculations

Orifice Flow Meters (FIC-115 and FIC-116)

Principle of Operation: The basis of the orifice flow meter calculation is defined by the following "practical working equation for weight rate of discharge, adopted by the ASME Research Committee on Fluid Meters for use with either gases or liquids," as quoted in *Perry's Chemical Engineers' Handbook* (6th Ed., Eqn. 5-14):

$$w = KYA_2\sqrt{2g_c(p_1 - p_2)\rho_1}$$

w = weight rate of discharge, lb/sec

K, Y are special coefficients, defined belowA_2 = cross sectional area of the orifice, ft^2

g_c = the gravitational constant (32.2 ft/sec^2)

p_1 = pressure at upstream static pressure tap, lb/ft^2

p_2 = pressure at downstream static pressure tap, lb/ft^2

ρ_1 = density of flowing fluid at upstream pressure and temperature, lb/ft^3

For the process control logic, the weight rate must be converted to "molar" or volumetric flow. The following equation applies:

$Q = w\,k\,/\,MW$

w = weight rate of discharge, lb/sec

k = conversion factor constants

MW is the molecular weight of the sample gas.

Application: The field instruments provide 3 measurements: the upstream gas temperature in degrees Fahrenheit (TE-115 and 116 for the regeneration offgas and coal gas loops, respectively), the upstream pressure in pounds per square inch (PT-115 and 116), and the pressure drop across the orifice in inches of water (PDT-115 and 116). With the appropriate conversion factors, these measurements can be plugged into the equation above.

Coefficients:

The K term is defined as follows:

$K = C/\sqrt{\ }(1-\beta^4)$, where

C = coefficient of discharge, dimensionless

β = ratio of the orifice diameter to the pipe diameter, dimensionless

C is the discharge coefficient and is empirically determined. From Figure 5-20 in Perry's, it appears that a typical value for the flow conditions that exist around the orifices on the DSRP skid should be 0.62.

β is the diameter ratio, and when raised to the fourth power, is a small number. Subtracting that value from 1.0, and then taking the square root results in a correction factor that is not much different from 1.0, so the algorithms that are programmed in the SCADA system ignore it. Similarly, the Y correction factor (for expansion of the gas across the orifice) is approximately 1.0 since this is a high pressure system with a very low orifice meter pressure drop. Thus, the KY term is approximately equal to C, which was stated above to be 0.62. This is an operator-adjustable term, as discussed in more detail below.

Constants:

A_2 comes from the mechanical design of the orifice. We have the following information about the orifice plates that are currently installed, but bear in mind that we may want to change out the plates, and enter new information into the calculation algorithms:

FE-115	Regenerable Offgas	0.2776 inches dia.	0.00042031 ft^2
FE-116	Coal Gas	0.1595 inches	0.00013875 ft^2

The $2g_c$ term is also a constant: 64.4 ft/sec^2.

Variables:

The DP transmitter directly measures the $(p_1 - p_2)$ term, except that the engineering units of the output (inches of water) has to have a conversion constant applied to get lb/ft^2 (multiply inches of water by 5.20).

The final step to complete the input to the mass flow calculation is to calculate the gas density. The gas density calculation utilizes the upstream pressure measurement, the gas temperature, and the molecular weight (MW). The molecular weight is not calculated continuously from field data; it is a keyboard input value and only needs to be changed by the operator if, during operation, the coal gas composition changes significantly from the design value.

The equation that applies is as follows:

$$\rho_1 = MW * P / (10.73 * (T + 459.6))$$

where ρ_1 is the density in lb/ft^3, P is the pressure in PSIA (the transmitter reading + 14.7), and T is the gas temperature in degrees Fahrenheit.

With the mass flow calculation complete, the final step is to convert the weight rate of discharge (*w*, calculated above) into volumetric (also called molar) flow. This calculation changes the units from "lb/sec" to "standard liters per minute" (SLPM) by applying the following equation:

w * (454 g/lb) * (60 sec/min) *(22.4 std L / mole) / (MW, g/mole) = w * 610,176 / MW

The calculated mass flow rate in SLPM becomes the "PV" or process value for feedback to the P-I-D controllers (FIC-115 and FIC-116, for regeneration off gas and coal gas respectively).

One final consideration in programming the mass flow calculation was providing the functionality to calibrate the orifice flow meter in the field by changing the value of the discharge coefficient. What the field crew successfully did during the commissioning activities was pass a known flow rate of nitrogen (measured in SLPM by an electronic mass flow controller) through the flow orifice and note the output value from the orifice meter calculations (after inputting the correct molecular weight). If the values did not match, the operator adjusted the orifice coefficient constant in order to force the values to match.

Stoichiometric Flow Ratio Calculation (FFC-260)

Principle of Operation: The flow ratio calculation starts with the output from the ROG orifice meter (FE-115) calculation, and applies a field instrument value to it to calculate the SO_2 component flow rate. Then the flow ratio controller applies a user-defined constant (the stoichiometric ratio; keyboard entry) to determine the required flow rate of the "reducing" components of the coal gas. Using two other field instrument values to define the current concentration of reducing components, the flow ratio controller determines the new set point for the coal gas flow controller (FIC-116).

Application: Figure A-1 diagrams the information flow for the flow ratio calculations that must be carried out to define the set point of the coal gas flow controller. Relevant equations are as follows:

$SO_2FLOW = ROGFLOW * \%SO_2$

$\%REDCOMP = \%H_2 + \%CO$

$REDCOMPF = STOICHR * SO_2FLOW$

$CGFLOW = REDCOMPF / \%REDCOMP$

where the terms, above, are defined as follows:

SO_2FLOW	Flow rate (in SLPM) of the sulfur dioxide component of the regeneration offgas.
ROGFLOW	Flow rate (in SLPM) of the regeneration offgas stream; output of the mass flow calculations of FIC-115
%SO_2	Volume % sulfur dioxide in the ROG; output of AIT-215.
%REDCOMP	% of reducing components of the coal gas.
%H_2	Volume % hydrogen in the coal gas; output of AR-240. [NOTE: this is a special signal and required special logical treatment, as described below.]
%CO	Volume % carbon monoxide in the coal gas; output of AIT-230.
REDCOMPF	Desired flow rate of reducing components (in SLPM).
STOICHR	The stoichiometric ratio of reducing components to SO_2; approximately equal to 2.0. THIS VALUE IS THE SET POINT OF FFC-260.
CGFLOW	Required coal gas flow to meet stoichiometry requirements. THIS VALUE IS THE OUTPUT OF FFC-260, and becomes the "floating" set point of FIC-116.

The data acquisition and processing of the signals for all of the above was quite straightforward, with the exception of the %H_2 signal. A gas chromatograph measures the hydrogen concentration (GC; AE-240). A GC is a "batch" device, in that it receives a small sample of the process gas (the "injection"), and then for a period of 20 or 30 minutes, passes that gas through a long, thin, heated (temperature-programmed) tube and past a detector. The detector generates a constantly varying voltage output that must have a considerable degree of signal processing in order to be made useful. A freestanding PC, running Hewlett-Packard Chemstations® software processes (*i.e.,* "integrates") that signal. Then a Labview® program extracts a single number – the H_2 concentration – from the Chemstation files, and outputs that number to a National Instruments analog-out board. That analog signal (4-20 mA) goes into the PLC of the DSRP control system. The whole combination of computer, two different software packages, and analog board is designated on the P&ID by the single bubble, AR-240.

The Labview® program generates a signal such that the H_2 concentration will have a fixed value for the duration of each sample. At the end of the injection, the integration calculations will take place, and a new H_2 concentration value will be calculated. That new value will be held for the duration of the next injection, and so on. During this time the carbon monoxide concentration in the coal gas could be changing, however, and the continuous CO analyzer will pick that up.

The concern in building a rugged control system for the field test, is that the GC can potentially (and, in fact, is somewhat likely to) generate spurious signals that will be integrated to give unlikely answers for the H_2 concentration. There is "error trapping" to check that the calculated value is reasonable, before letting FFC-260 use that value in a fully automatic mode to determine the new value for the set point for the coal gas flow rate.

The overall process control has three levels of automatic control, as follows:

MANUAL	Valves FCV-115 and FCV-116 will have their position determined by the operator inputting "% open" values into FIC-115 and 116.
SEMI-AUTOMATIC	The PID loops for FCV-115 and FCV-116 will be operational, with the mass flow calculations operating, so that the operator can input a set point value (in SLPM) and the valve controller will strive to maintain that value. This mode of operation is equivalent to turning OFF the FFC-260. In this mode, the FFC-260 calculations will continue to be displayed on the screen, for de-bugging purposes, but the set point of FIC-116 will not be changed.
FULL AUTOMATIC	The stoichiometric flow ratio controller (FFC-260) is turned ON, and the coal gas set point is constantly modulated in response to the changing compositions of the ROG and CG so that the ratio of reducing gas components to the SO2 content is equal to the set point.