INTRODUCTION

This document explains the signal processing required to linearise, temperature compensate and calibrate all SGX Sensortech infrared gas sensors, followed by the calculations required to determine the concentration of the target gas.

External circuit/software will be required to perform the signal processing and to store calibration information (in non-volatile memory). See Infrared Sensor Application Notes 3 and 4.

An example of each calculation is shown using typical values.

SENSOR OUTPUTS

The output signals for the gas sensors consist of the following:

Active Detector(s): Sinusoidal output at the same frequency as the lamp pulses. The amplitude of this signal decreases when the target gas is present.

Reference Detector: Sinusoidal output at the same frequency as the lamp pulses. This detector is used to compensate for changes in source intensity, optical degradation and temperature to some degree. The amplitude of this device will not show any changes due to the effects of the target gas.

Thermistor: An output relating to the temperature of the device, requiring further linearisation (see Temperature Measurements, page 5).

Temperature Sensor: A linearised DC output relating to the temperature of the device.

Note: Not available in all sensors.

TARGET GAS CONCENTRATION CALCULATION OVERVIEW

The outputs of the Active and Reference detectors must be monitored continuously to obtain their peak-to-peak outputs. The target gas concentration is calculated from the ratio of these outputs (normally averaged) performed at regular intervals (i.e. every second). When installed the sensors will require the calculation of the Zero and Span values (calibration), which must be stored in the non-volatile memory for future use. Linearisation is performed during the calculation using the “a” and “n” coefficients (see Appendix G), and is based upon the Beer-Lambert Law.

The following information shows step-by-step instructions to determination the target gas concentration. Compensation will be required to remove the effects of temperature. This is performed on the Normalised Ratio, calculated from the sensor output measurements (known as the alpha compensation) and on the Span (known as the beta compensation) obtained during the calibration routine.

Note: Normalised Ratio = Act / (Zero x Ref)
Normalised Absorbance = 1 - (Act / (Zero x Ref))

<table>
<thead>
<tr>
<th>Gas</th>
<th>Alpha</th>
<th>Beta</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>No*</td>
<td>Yes</td>
</tr>
<tr>
<td>Hydrocarbons</td>
<td>Yes</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Table 1 - Temperature Compensation Requirements

* Alpha compensation can be used for increased accuracy over the concentration range.

Figure 1 overleaf shows the process to determine the temperature compensated target gas concentrations for both CO2 and hydrocarbon devices.
CALIBRATION

The calibration routine of the infrared gas sensor calculates “Zero” and “Span” used during the calculation of the target gas concentration. These values must be stored in non-volatile memory (so the values still remain when the power to the device is removed). The temperature at the time of calibration ($T_{cal}$) must be measured and stored with the Zero and Span readings in the non-volatile memory for future use during temperature compensation calculations.

a.) Calculate the “Zero”

The following calculation is performed when the gas sensor is being exposed to the zero test gas (i.e. nitrogen), without the presence of the target gas.

$$\text{Zero} = \frac{\text{Act}}{\text{Ref}}$$

Where:
- Act = the peak-to-peak output of the Active Detector in volts in zero test gas.
- Ref = the peak-to-peak output of the Reference Detector in volts in zero test gas.

b.) Calculate the “Span”

The following calculation is performed when the gas sensor is being exposed to the calibration test gas.

$$\text{Span} = \left[1 - \frac{\text{Act}}{\text{Zero} \times \text{Ref}}\right] \div \left[1 - \exp(-aC^n)\right]$$

Where:
- Act = the peak-to-peak output of the Active Detector in volts in the calibration test gas.
- Ref = the peak-to-peak output of the Reference Detector in volts in the calibration test gas.
- Zero = the “Zero” value (stored in non-volatile memory) calculated during this calibration routine.
- $a$ = fixed linearisation coefficient (see Appendix G).
- $C$ = the concentration of the applied calibration test gas in % Volume (i.e. 5 for 5% Vol.).
- $n$ = fixed linearisation coefficient (see Appendix G).
TEMPERATURE COMPENSATION

The use of the ratio of active and detector signals provides, in addition to independence of lamp intensity, a level of temperature compensation. However, the effect of temperature on the detector signals is complex and varies between different sensor types.

The major effect on the hydrocarbon channel is a change in apparent zero level with temperature, which is compensated using the alpha temperature compensation. If not corrected, this results in an almost linear positive shift in baseline with an increase in temperature. The major effect on the CO$_2$ channel is the apparent change in span with temperature, which is compensated using the beta temperature compensation.

It is recommended that the alpha and beta coefficients are split into two ranges, assuming the value of $T_{cal}$ is close to 20 °C:

i.) Negative (of $T_{cal}$) temperature compensation (“alphaneg” & “betaneg”)

ii.) Positive (of $T_{cal}$) temperature compensation (“alphapos” & “betapos”)

a.) Alpha Temperature Compensation

The alpha coefficient can either be entered as a fixed coefficient derived from experimental testing or recalculated “interactively” in the software (HC devices only) to ensure that the sensor-to-sensor variations in the alpha coefficient are minimised (See Interactive Alpha Calculation Method below).

Normalised Ratio $(_{\text{comp}})$ = Normalised Ratio x $(1 + \alpha (T - T_{cal}))$

Where:
- Normalised Ratio = Act / (Zero x Ref)
- Act = the peak-to-peak output of the Active Detector in volts.
- Zero = the “Zero” value (stored in non-volatile memory) calculated during the calibration routine (see Calibration above).
- Ref = the peak-to-peak output of the Reference Detector in volts.
- $\alpha$ = the “alpha” coefficient, either “alphapos” or “alphaneg” (see Appendix G),
- $T$ = the actual temperature measured at the sensor in kelvin.
- $T_{cal}$ = the temperature (stored in non-volatile memory) measured during the calibration routine (see Calibration above) in kelvin.

b.) Beta Temperature Compensation

The Beta temperature compensation relates to the apparent change in “Span” over temperature. The coefficient is entered as a fixed value.

Span$(_{\text{comp}})$ = Span + ($\beta \times ((T – T_{cal}) / T_{cal}))$

Where:
- Span = the “Span” value (stored in non-volatile memory) calculated during the calibration routine (see Calibration above).
- $\beta$ = the “beta” coefficient, either “betapos” or “betaneg” (see Appendix G).
- $T$ = the actual temperature measured at the sensor in kelvin.
- $T_{cal}$ = the temperature (stored in non-volatile memory) measured during the calibration routine (see Calibration above) in kelvin.

c.) Calculation of the Target Gas Concentration

$C = \left(–\ln\left[1 – \frac{(1 – \text{Normalised Ratio }(_{\text{comp}}))}{\text{Span}(_{\text{comp}})}\right]\right) / a(1 / n)$

Where:
- $a$ = fixed linearisation coefficient (see Appendix G).
- $n$ = fixed linearisation coefficient (see Appendix G).

Note: For this equation to work the value of “$(1 – \text{Normalised Ratio }(_{\text{comp}}))$” needs to be positive. If a negative value is obtained then perform the following actions if required:

(i) Convert $(1 – \text{Normalised Ratio }(_{\text{comp}}))$ to a positive value (i.e. multiply by “–1”, known as the modulus).
(ii) Perform the calculation to determine concentration, as normal.
(iii) Display the concentration as a negative value (i.e. multiply by “–1”).

This is the same as the following equation:

$C = –\left(\ln\left[1 – \frac{(1 – \text{Normalised Ratio }(_{\text{comp}}))}{\text{Span}(_{\text{comp}})}\right]\right) / a(1 / n)$
INTERACTIVE ALPHA CALCULATION METHOD

This section describes the use of an “interactive” method to determine the alpha coefficient for the gas sensor, which has been installed, by recalculating the alpha coefficient via the software. This may be required to minimise the inherent sensor-to-sensor variations in the alpha coefficient. The theory behind this method is that it is assumed that a Normalised Ratio of > 1.00 is due to temperature as this is equivalent to a negative gas concentration.

The temperature compensation works by initially setting default alpha (\(\alpha\)) coefficients. The compensation is split into two regions, both of which will have their own \(\alpha\) coefficients (“alphaneg” and “alphapos”):

i.) Negative (of \(T_{cal}\)) temperature compensation (“alphaneg”)

ii.) Positive (of \(T_{cal}\)) temperature compensation (“alphapos”)

The suggested default alpha values set up in the start-up routine of the software are as follows:

“alphaneg” = 0.0000
“alphapos” = 0.0010 (Set high enough to force overcompensation (and therefore alpha recalculation) if positive temperature change is seen, but not too high to mask the response to the target gas).

There are two conditions that need to be met in order to recalculate the alpha value:

i.) The difference between the current temperature and the calibration temperature is >5 °C.

ii.) Whenever the Normalised Ratio (for “alphaneg”) or Normalised Ratio (\(\text{comp}\)) (for “alphapos”) readings increase to greater than the max value from the previous alpha recalculations (i.e. the \(\alpha\) will be recalculated initially if the reading is >1.00 (say it goes to 1.01), and further recalculations will only occur if the reading increases to greater than 1.01 and so on.

The graph below shows the uncompensated, overcompensated (using default “alphapos”) and the ideal Normalised Ratio whilst being exposed to the zero test gas. The y-axis = Normalised Ratio.

![Diagram showing uncompensated, overcompensated, and ideal Normalised Ratio.]

Note: A possible situation could arise whereby, after initial set-up, the sensor is exposed to a certain level of target gas while still using the default \(\alpha\). If this occurs and the temperature increases then the overcompensated reading would be lower due to the shift downwards in Normalised Ratio (i.e. could be reading 1.01 instead of its true 1.05, due to a response of 0.04, which will cause the display to reading a concentration of gas lower than the actual. Once the gas is removed from the sensor, then the (Act/(Zero*Ref)) will go back to the true zero, while this is happening the reading will increase and will try to get back to the true zero of 1.05. But each time the max reading is exceeded, alpha will be recalculated until eventually the true zero will be found and compensated for. It is essential that the default value of “alphapos” is not too high to mask too much response to gas.

The general equation used for the temperature compensation is:

\[
\text{Normalised Ratio (comp)} = \text{Normalised Ratio} \times (1 + \alpha (T - T_{cal}))
\]

which is rearranged to give:

\[
\alpha = ((\text{Normalised Ratio (comp)} / \text{Normalised Ratio}) - 1) / (T - T_{cal})
\]

Where:

- Normalised Ratio (comp) = Target compensated value (= 1.00 equivalent to 0% vol.)
- Normalised Ratio = Current uncompensated value
- \(T\) = Current temperature in Kelvin
- \(T_{cal}\) = Temperature at point of “Calibration of Zero” in Kelvin.
TEMPERATURE MEASUREMENTS

Thermistor
The signal from the thermistor can be converted to temperature using the following appropriate third order polynomial equation:

Temperature (K) = \(375.120 - (54.122 \times V) + (13.349 \times V^2) - (1.617 \times V^3)\)
(Twin Gas Devices only, e.g. IRxxTT)

Temperature (K) = \(395.47 - (74.94 \times V) + (19.68 \times V^2) - (2.327 \times V^3)\)
(IRxxEx Devices only)

Where \(V\) = voltage between the 10 \(\Omega\) resistor and the thermistor output (see Infrared Sensor Application Note 4).

Temperature Sensor
The signal from the temperature sensor can be converted to temperature using the following equation:

Temperature (K) = \(((V - 0.5) / 0.01) + 273\)
(IR600 Series Devices only)

Temperature (K) = \(((V - 0.424) / 0.00625) + 273\)
(IRxxGx Devices only)

Where \(V\) = voltage output of the temperature channel.
APPENDIX A – EXAMPLE OF ZERO CALCULATION

\[ \text{Zero} = \frac{\text{Act}}{\text{Ref}} \]

If:
\begin{align*}
\text{Act} &= 1.60 \text{ V (typical active peak-to-peak reading).} \\
\text{Ref} &= 1.20 \text{ V (typical reference peak-to-peak reading).}
\end{align*}

Note: For single channel devices this value can be fixed to 1.00 in software.

Therefore:
\[ \text{Zero} = \frac{1.60}{1.20} = 1.33 \]

APPENDIX B – EXAMPLE OF SPAN CALCULATION

\[ \text{Span} = 1 - \frac{\text{Act}}{(\text{Zero} \times \text{Ref}) / \exp(-a \times C^n)} \]

The following example shows the possible readings obtained when an infrared sensor is exposed to 2% vol. calibration gas. The active peak-to-peak voltage will decrease as the gas is applied. So if:
\begin{align*}
\text{Act} &= 1.12 \text{ V (decreased active peak to peak voltage drop);} \\
\text{Ref} &= 1.20 \text{ V (no change will be seen from peak-peak reading in nitrogen);} \\
\text{Zero} &= 1.33 \text{ (value stored from “Calibration of Zero” in non-volatile memory);} \\
a &= 0.672 \text{ (fixed linearisation coefficient - see Appendix G);} \\
n &= 0.746 \text{ (fixed linearisation coefficient - see Appendix G);} \\
C &= 2 \text{ (known concentration of calibration gas 2% vol.)}
\end{align*}

Therefore:
\[ \text{Span} = 1 - \frac{1.12}{(1.33 \times 1.20)} / \exp(-0.672 \times 2^{0.746}) \]
\[ = \frac{0.298}{0.676} \]
\[ = 0.4408 \]

APPENDIX C – EXAMPLE OF ALPHA CALCULATION

\[ \text{Normalised Ratio (comp)} = \text{Normalised Ratio} \times (1 + \alpha (T - T_{\text{cal}})) \]

Where:
\[ \text{Normalised Ratio} = \frac{\text{Act}}{(\text{Zero} \times \text{Ref})} \]

If:
\begin{align*}
\text{Act} &= 1.45 \text{ V (stable peak-to-peak reading in unknown target gas concentration);} \\
\text{Ref} &= 1.30 \text{ V (reference peak-to-peak reading in unknown target gas concentration);} \\
\text{Zero} &= 1.33 \text{ (value stored from “Calibration of Zero” in non-volatile memory);} \\
\alpha &= 0.000556 \text{ (typical “alpha” value reading);} \\
T_{\text{cal}} &= 293 \text{ K (20 °C) (temperature stored in non-volatile memory, from calibration routine);} \\
T &= 313 \text{ K (40 °C) (current temperature).}
\end{align*}

Therefore:
\[ \text{Normalised Ratio (comp)} = \frac{1.45}{(1.30 \times 1.33)} \times (1 + 0.000556 \times (313 - 293)) \]
\[ = 0.8386 \times 1.0111 \]
\[ = 0.8480 \]

APPENDIX D – EXAMPLE OF BETA CALCULATION

\[ \text{Span(comp)} = \text{Span} + [\beta \times ((T - T_{\text{cal}}) / T_{\text{cal}})] \]

If:
\begin{align*}
\text{Span} &= 0.4408 \text{ (value stored in non-volatile memory, from calibration routine);} \\
\beta &= 0.838 \text{ (example beta temperature coefficient - see Appendix G);} \\
T_{\text{cal}} &= 293 \text{ K (20 °C) (temperature stored in non-volatile memory, from calibration routine);} \\
T &= 313 \text{ K (40 °C) (current temperature).}
\end{align*}

Therefore:
\[ \text{Span_{comp}} = 0.4408 + (0.838 \times (313 - 293) / 293) \]
\[ = 0.4408 + 0.0572 \]
\[ = 0.4980 \]
APPENDIX E – EXAMPLE OF TARGET GAS CONCENTRATION CALCULATION

\[ C = ( -\ln \left( 1 - \frac{(1 - \text{Normalised Ratio}_{\text{comp}})}{\text{Span}_{\text{comp}}} \right) / a )^{1/n} \]

If:
- Normalised Ratio_{\text{comp}} = 0.848;
- \text{Span}_{\text{comp}} = 0.4765;
- a = 0.672 (Fixed linearisation coefficient - see Appendix G);
- n = 0.746 (Fixed linearisation coefficient - see Appendix G).

Therefore:

\[ C = \left( -\ln \left( 1 - \frac{(1 - 0.848)}{0.4980} \right) / 0.672 \right)^{1/0.746} \]
\[ = \left( -\ln \left( \frac{0.6947}{0.672} \right) \right)^{1.340} \]
\[ = \frac{0.3643}{0.672} \]
\[ = 0.44 \% \text{ vol.} \]

APPENDIX F – EXAMPLE OF INTERACTIVE ALPHA GENERATION METHOD

\[ \alpha = \frac{(\text{Normalised Ratio}_{\text{comp}} / \text{Normalised Ratio}) - 1}{(T - T_{\text{cal}})} \]

If, after set-up, the temperature decreases from the calibrated temperature, the uncompensated Normalised Ratio will be >1.00. This will then trigger the recalculation of the alpha (“alphaneg”) constant.

\[ \alpha = \frac{(1.00 / 1.01) - 1}{(273-293)} \]
\[ = \frac{0.99}{20} \]
\[ = 0.00495 \text{ (alphaneg)} \]

“alphaneg” and new highest uncompensated Normalised Ratio (= 1.01) is then stored in memory. The software now uses the new “alphaneg”, for all readings < \( T_{\text{cal}} \), and continually monitors the Normalised Ratio to check that the value does not exceed the new highest uncompensated reading. If this value is exceeded then alpha needs to be recalculated.

If, after set-up, the temperature increases from the calibrated temperature, the Normalised Ratio_{\text{comp}}, overcompensated reading will be >1.00, due to the high default “alphapos”. This will trigger the recalculation of the \( \alpha \) (“alphapos”) constant.

\[ \alpha = \frac{(1.00 / 0.99) - 1}{(313-293)} \]
\[ = \frac{0.01}{20} \]
\[ = 0.000505 \text{ (alphapos)} \]

“alphapos” and new highest compensated Normalised Ratio (= 1.01) is then stored in memory. The software now uses the new “alphapos”, for all readings > \( T_{\text{cal}} \), and continually monitors the Normalised Ratio_{\text{comp}} reading to check that the value does not exceed the new highest compensated reading. If this value is exceeded then alpha needs to be recalculated.

Note: The new highest compensated Normalised Ratio is not stored if triggered by the default value overcompensation (i.e. the first instance that “alphapos” is recalculated).
APPENDIX G – TABLE OF COEFFICIENTS

Note: These coefficients are based upon results measured at SGX Sensortech using standard test equipment. These coefficients may vary slightly when using different circuits. It may be required to recalculate some of these coefficients if small inaccuracies are observed during testing (refer to Infrared Sensor Application Note 5 for determination of coefficients).

Note: For sensor variants with a "1" suffix (supported lamp versions), use the equivalent non-supported lamp version. For example for an IR11GM_1, use coefficients for the IR11GM.

<table>
<thead>
<tr>
<th>Sensor Type</th>
<th>Gas Type</th>
<th>Range (v/v)</th>
<th>a</th>
<th>n</th>
<th>alpha</th>
<th>anom</th>
<th>betap</th>
<th>betan</th>
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</thead>
<tbody>
<tr>
<td>IR11BD / IR21BD</td>
<td>CO₂</td>
<td>0.5%</td>
<td>2.49</td>
<td>0.811</td>
<td>0.000464</td>
<td>0.0000501</td>
<td>0.084</td>
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<td>1.12</td>
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<td>0.0000501</td>
<td>0.084</td>
<td>0.143</td>
<td></td>
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<td>IR11BD / IR21BD</td>
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<td>0.892</td>
<td>0.570</td>
<td>0.0000501</td>
<td>0.084</td>
<td>0.143</td>
<td></td>
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<td>1.88</td>
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<td>0.000242</td>
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<td>IR12BD / IR22BD</td>
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<td>IR13BD / IR23BD</td>
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<td>-0.164</td>
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<td>-0.059</td>
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<td>IR15TT-M / IR25TT-M</td>
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<td>IR15TTR-R</td>
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<td>0.542</td>
<td>0.000586</td>
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SGX Sensortech (IS) Ltd Registered in England No. 08067077 A1A-Infrared_AN2 Version 2, page 8
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