



# **Application Notes**

# **Using KEMET NDIR Gas Sensors**

# Linear Approximation from I<sup>2</sup>C Data Registers

The above information is believed to be correct but does not purport to be all inclusive and must be used only as a guide.

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## **TABLE OF CONTENTS**

1	INTRO	DUCTION	3
2	GETTII	NG TO KNOW THE I <sup>2</sup> C GAS DETECTOR	3
	2.1	Assuming the Use of a Reference Channel within the Gas System	3
	2.2	Interpolating Values in the Gas System	4
	2.3	Method to Linearise Gas Prediction	5
3	EXCEL	SPREADSHEET SOLVER ADD-IN	7
	3.1	Installing the Solver	7
	3.2	Using the Solver	8
	3.3	Finalizing the Linear Prediction	10

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### **1** INTRODUCTION

This application note is about interpolating the data from KEMET's SMD I<sup>2</sup>C devices and shows a method of creating an Excel spreadsheet and then using Excel Add-ins to solve a linear curve approximation.

This document acts as a user reference guide and should be used alongside the Excel spreadsheet *KEMET NDIR Gas Linearisation.xlsx*. It guides the reader through using the register values during the calibration process and details the methodology on how to use a modified Beer Lambert equation to interpolate the registers and thus demonstrate the difference between **transmission** and **absorption** and showing that both curves are non-linear. It will also provide methods on how to use equations and solvers to linearise results, explaining how to install the necessary Add-ins into an Excel spreadsheet and then a step by step guide on how the Excel spreadsheet values change when the solver function is used to find the best linear fit.

## 2 GETTING TO KNOW THE I<sup>2</sup>C GAS DETECTOR

#### 2.1 Assuming the Use of a Reference Channel within the Gas System

The Beer-Lambert Law, stating that the loss of light intensity when propagated in a medium is directly proportional to intensity and path length, implies that the curve is non-linear. In our case it relates to the IR being transmitted and the gas in which that IR is being transmitted through.

Practical NDIR applications require the following modified Beer-Lambert Law:



$$T = a(1 - e^{-bx^c})$$

Figure 1 – Example Register Values

In most systems a reference channel is used to determine the transmission intensity, which takes also into consideration the transmission path length. A gas channel determines the transmission attenuation due to the presence of gas. Many engineers use the term **absorption** instead of the term "transmission attenuation".

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### 2.2 Interpolating Values in the Gas System

First, calculate and populate the Ratio column for each Gas %.

To do so, let's use the data from Table 1, and divide the Gas Sensor data (Io) by the Reference Sensor data (I), the result we will call the **Ratio**.

Calculate Transmittance T values by using Ratio value for each Gas %.

To do this and divide by **Ratio** value for each gas percentage by the value for **0%** gas.

	Actual Cas %	Reference	Gas	Ratio	Transmittance	Absorption	
	Actual Gas %	Sensor (I)	Sensor (Io)	Gas / Ref	(T)	(1-T)	
	0	21903	27976	1.277268	1.000000	0.000000	
	10	21931	27510	1.254799	0.982409	0.017591	( Absorption )
1.000 - 1.277	20	21020	27065	1.234210	0.966289	0.033711 🧲	
$1.000 = \frac{1.277}{1.277}$	20	21950	26681	1.215535	0.951668	0.048332	1 – T values
1 2 5 4	40	21933	26322	1.200109	0.939591	0.060409	
$0.982 = \frac{1.231}{1.277}$	50	21945	25987	1.184188	0.927126	0.072874	
1.277	60	21961	25744	1.172260	0.917787	0.082213	
	70	21971	25546	1.162714	0.910314	0.089686	
	80	21978	25347	1.153290	0.902935	0.097065	
	90	21982	25205	1.146620	0.897713	0.102287	
	100	21971	25068	1.140959	0.893280	0.106720	

Table 1 – Calibration Data

Using values calculated for **Transmittance** (see Table 1), transmittance can now be plotted. We can see in Figure 2 that the resultant graph is <u>non-linear</u>.



Figure 2 – Transmittance Curve

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Using the formula (**1-T**), it is possible to calculate the values for **Absorption**. Plotting the curve of absorption of Figure 3, we can also see the resultant graph is <u>non-linear</u>.



Figure 3 – Absorption Curve

## 2.3 Method to Linearise Gas Prediction

Using the modified Beer-Lamberts equation allows us to predict more accurately offsets within the system (see equation PA below). The Microsoft Excel spreadsheet solver function enables the user to use an iterative process to estimate the best values for linearisation (see equation X below).

To do so, the Excel spreadsheet needs to include the Add-ins, and the Solver function.



Modify the Excel spreadsheet to include the following:

- Add a new column called **Predicted Absorption (PA)**: this column will calculate values using the equation PA.
- Add a new column called Linearised Gas % (X): this column will calculate values using the equation X.
- Add a new column called **SQRD Delta (R<sup>2</sup>)**: the numeric value of R<sup>2</sup> is used by the Excel Solver to linearise the final gas prediction.

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Each numeric expression is written into the three new columns. The Excel Solver functions, and initial variables, have been written into the table below:

		Example (	Calibration Da	ata						
Actual Gas (%)	Reference Sensor (I)	Gas Sensor (lo)	Ratio Gas / Ref	Transmittanc e (T)	Absorption (A) = '1-T'	Predicted Absorption (PA)	Linearised Gas % (X)	SQRD Delta (R <sup>2</sup> )	Modified Beer-Lambert Equation (PA)	Linearised Gas Equation (X)
0	21903	27976	1.277268	1.000000	0.000000	0.000000	0	0.00E+00		
10	21931	27519	1.254799	0.982409	0.017591	0.397130	0.005131267	1.44E-01		
20	21929	27065	1.234210	0.966289	0.033711	0.446561	0.019489142	1.70E-01		
30	21950	26681	1.215535	0.951668	0.048332	0.467670	0.041339215	1.76E-01		
40	21933	26322	1.200109	0.939591	0.060409	0.478835	0.066320092	1.75E-01	in the second	$c \ln \left(1 - \frac{ABS}{2}\right)$
50	21945	25987	1.184188	0.927126	0.072874	0.485428	0.099262959	1.70E-01	$ABS = a(1 - e^{-bx^2})$	$u = \binom{m}{1} a$
60	21961	25744	1.172260	0.917787	0.082213	0.489602	0.129076918	1.66E-01	. ,	$x = \sqrt{-h}$
70	21971	25546	1.162714	0.910314	0.089686	0.492376	0.156319282	1.62E-01		$\sqrt{-b}$
80	21978	25347	1.153290	0.902935	0.097065	0.494289	0.186336222	1.58E-01		
90	21982	25205	1.146620	0.897713	0.102287	0.495646	0.209539871	1.55E-01		
100	21971	25068	1.140959	0.893280	0.106720	0.496631	0.230563309	1.52E-01		
										Variable 'a' 0.50000
									$R^2 = 1.63E+00$	Variable 'b' 0.50000
										Variable 'e' 0.50000

- Using initial values of 0.5 for each variable 'a', 'b' and 'c'.
- PA and X columns are automatically populated with **estimated** values.
- Notice also that the sum of the Delta R<sup>2</sup> column has now been calculated as 1.63. This value is part of the solver function and <u>must not</u> be manually modified.

Each time a solver iteration is conducted, these values will subsequently change.

When variables 'a', 'b' and 'c' no longer change, this means these unchanged values are the **best** approximation (no more than three iterations should be required using the Solver).

From this process, the linearisation process and results can be calculated and proved:



Figure 4 – Linearized Gas Prediction

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#### 3 **EXCEL SPREADSHEET SOLVER ADD-IN**

#### **Installing the Solver** 3.1

Follow these simple steps to install and run the Solver function from Excel:

Within Excel spreadsheet, click File, and then click on Options in the green menu. •



Scroll to the bottom of the list and click on **Add-ins**. •



Select Solver Add-in, Then click OK.





Within an Excel spreadsheet, select the menu item called Data,



You will now see a new function called SOLVER, • this is the new function you will use to calculate the linearization variables.



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#### 3.2 Using the Solver

Open the Excel spreadsheet intended to be used for the gas calibration process.

- Within the spreadsheet, identify and name four cells that will be used for the linearisation solver.
- In below example, the first cell is called R<sup>2</sup>.
- The remaining cells are then identified as Variable 'a', Variable 'b' and Variable 'c'.

In the example, they are cell locations	\$L\$16 \$0\$1	5 \$0\$16	sos
	Variable 'c'	1.08839	
$R^2 = 1.83E-06$	Variable 'b'	0.01149	
	Variable 'a'	0.13024	

• Remember Cell locations as they will be required by the **Solver** function.

Initial variable conditions should be set to 0.5 and ensure R<sup>2</sup> value is at 1.63.

	Variable 'a'	0.50000
$R^2 = 1.63E+00$	Variable 'b'	0.50000
	Variable 'c'	0.50000

Click on the Solver icon within the Data menu, to open the Solver Parameters dialog box.



The objective is identified as the result of the R<sup>2</sup> Cell.

Variable cells are identified as Variable 'a', 'b' and 'c'.

The method used to solve the linearisation is **GRG Nonlinear**.

Make sure the four cells you identified in the previous step are correctly identified within the **Solver Parameters**.

So	Iver Parame	ters				×
	Se <u>t</u> Objecti	ve:		\$L\$16		Ì
	To: <u>By Changin</u>	O <u>M</u> ax q Variable Cells:	Mi <u>n</u>	O <u>V</u> alue Of:	0.99	
	\$Q\$15:\$Q\$	17				±
	Subject to	the Constraints:				
					~	
	🗹 Ma <u>k</u> e U	Jnconstrained Va	ariables Non-N	Vegative		
	S <u>e</u> lect a So Method:		5 Nonlinear		~	O <u>p</u> tions
	Solving	Method				
	Select t engine non-sm	he GRG Nonline for linear Solver tooth.	ar engine for S Problems, and	Solver Problems that d select the Evolution	are smooth nonlinear. Se ary engine for Solver pro	lect the LP Simplex oblems that are
	<u>H</u> elp			<	<u>S</u> olve	Cl <u>o</u> se

#### Now simply click Solve.

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Assuming the original data set within the excel file provided is being used

- the R<sup>2</sup> value as well as the Variables 'a', 'b' and 'c' should all have changed as per below:
- Linearized Gas %
- Predicted Absorption
- SQRD Delta

All NEW values are now calculated by the Solver process.

Predicted Absorption (PA)	Litearised Gas ( (X)	i QRD Delta (R)	Modified Beer-Lambert Equation (PA)	Linearised Gas Equation (X)
0.000000 0.021478 0.036165 0.048670 0.059790 0.069890 0.079183 0.087809 0.095866 0.103428	0 7.699770142 18.19376017 29.71221284 40.58778633 53.12614296 63.43171972 72.27205252 81.54578391 88.45208617	0.00E+00 1.51E-05 6.02E-06 1.14E-07 3.84E-07 8.91E-06 9.18E-06 3.52E-06 1.44E-06 1.30E-06	$ABS = a \left( 1 - e^{-bx^c} \right)$	$x = \sqrt[c]{\frac{\ln\left(1 - \frac{ABS}{a}\right)}{-b}}$
0.110553	91.5479639	1.47E-05	R <sup>2</sup> = 6.07E-05	Variable 'a' 0.30725 Variable 'b' 0.01177 Variable 'c' 0.78920

Values for R<sup>2</sup>, Variable 'a', Variable 'b', and Variable 'c' all changed.

	Solver Results	×
	Solver encountered an error value in the a Constraint cell.	Objective Cell or Reports
If or when the <b>Solver</b> shows the	<ul> <li><u>Keep Solver Solution</u></li> <li><u>Restore Original Values</u></li> </ul>	
following message just click OK.	Return to Solver Parameters Dialog	O <u>u</u> tline Reports
	<u>O</u> K <u>C</u> ancel	<u>S</u> ave Scenario
	Solver encountered an error value One of the cells in the worksheet be when Solver tried certain values fo	in the Objective Cell or a Constraint cell. came an error value r the Variable Cells.

- click the Solver icon a second time, and the values in the tables will change again.
- Click the **Solver** icon a third time, yet again the values in the tables will change.
- Linearized Gas %
- Predicted Absorption
- > SQRD Delta

All NEW values are now calculated by the Solver process



Values for R<sup>2</sup>, Variable 'a', Variable 'b', and Variable 'c' all changed.

- Solution found.
- If none of the values within those identified cells change from the previous iteration, then the **Solver** has computed the best variables for the linear approximation.



#### 3.3 Finalizing the Linear Prediction

In the table below we can see no values have changes from the previous solver iteration, we
can now use these numbers as the values for our Modified Beer-Lambert and Linearization
equations.

Predicted Absorption (PA)	Linearised Gas % (X)	SQRD Delta (R <sup>2</sup> )	Modified Beer-Lambert Equation (PA)	Linearised Gas Equation (X)
0.000000	0	0.00E+00		
0.017108	10.27876593	2.33E-07		
0.033703	20.00500611	6.20E-11		
0.048478	29.89418513	2.14E-08		( ADS)
0.061341	39.22344435	8.69E-07	( huf)	$c \ln \left(1 - \frac{ABS}{2}\right)$
0.072405	50.46091829	2.20E-07	$ABS = a(1 - e^{-bx^2})$	(n(1 a))
0.081845	60.42545327	1.36E-07		$x = \sqrt{\frac{-h}{-h}}$
0.089851	69.77672779	2.71E-08		$\sqrt{\sqrt{-D}}$
0.096610	80.73917427	2.07E-07		
0.102296	89.98372751	7.17E-11		
0.107062	99.21847457	1.17E-07		
				Variable 'a' 0.13024
			$P^2 = 1.83E-06$	Variable 'b' 0 01149
			R = 1.03E-00	
				Variable 'c' 1.08839

If we can use these new variables, we can plot the resultant linearized graph. The result of calculating the three variables for Beer-Lambert Law yields the following **Linearisation**.



Figure 5 – Linearised Gas Prediction and Trend Line

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