Application Notes

Using KEMET NDIR Gas Sensors

Linear Approximation from I²C Data Registers

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DOCUMENT HISTORY

Version	Date	Change Ref.	Change Details
01	25 MAR 2021	N/A	First Release

1 INTRODUCTION

This application note is about interpolating the data from KEMET's SMD I²C 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 I²C 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:

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

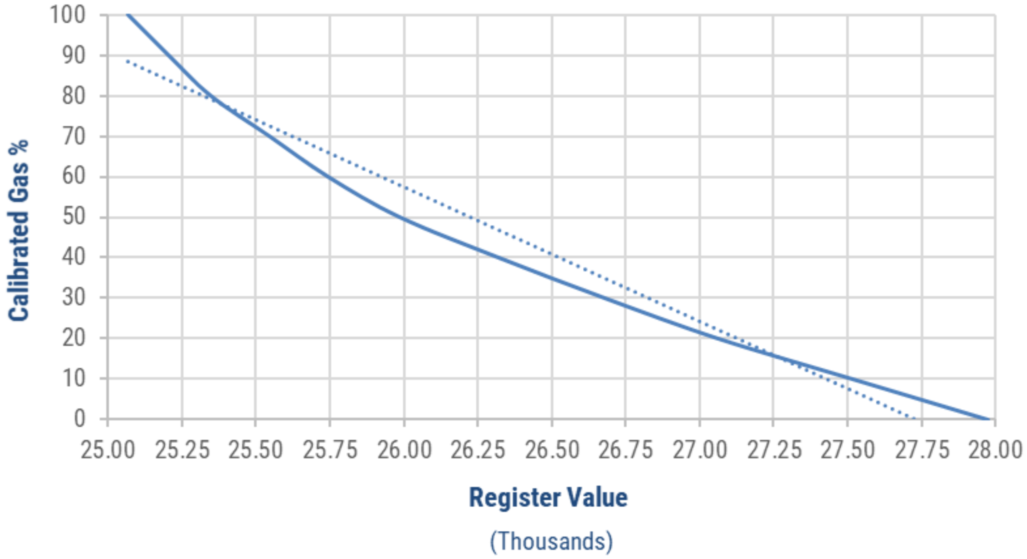


Figure 1 – Example Register Values

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".

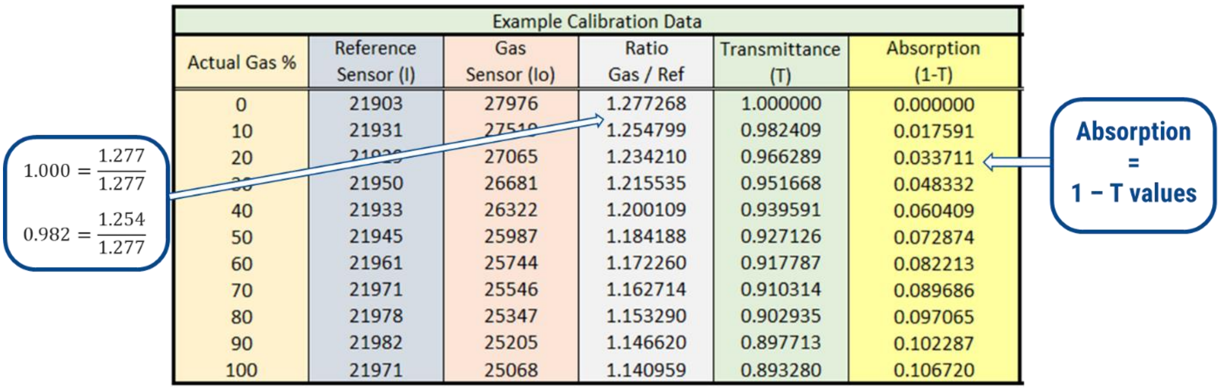
2.2 Interpolating Values in the Gas System

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.



$$1.000 = \frac{1.277}{1.277}$$

$$0.982 = \frac{1.254}{1.277}$$

Example Calibration Data

Actual Gas %	Reference Sensor (I)	Gas Sensor (Io)	Ratio Gas / Ref	Transmittance (T)	Absorption (1-T)
0	21903	27976	1.277268	1.000000	0.000000
10	21931	27519	1.254799	0.982409	0.017591
20	21929	27065	1.234210	0.966289	0.033711
30	21950	26681	1.215535	0.951668	0.048332
40	21933	26322	1.200109	0.939591	0.060409
50	21945	25987	1.184188	0.927126	0.072874
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

Absorption = 1 – T values

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>.

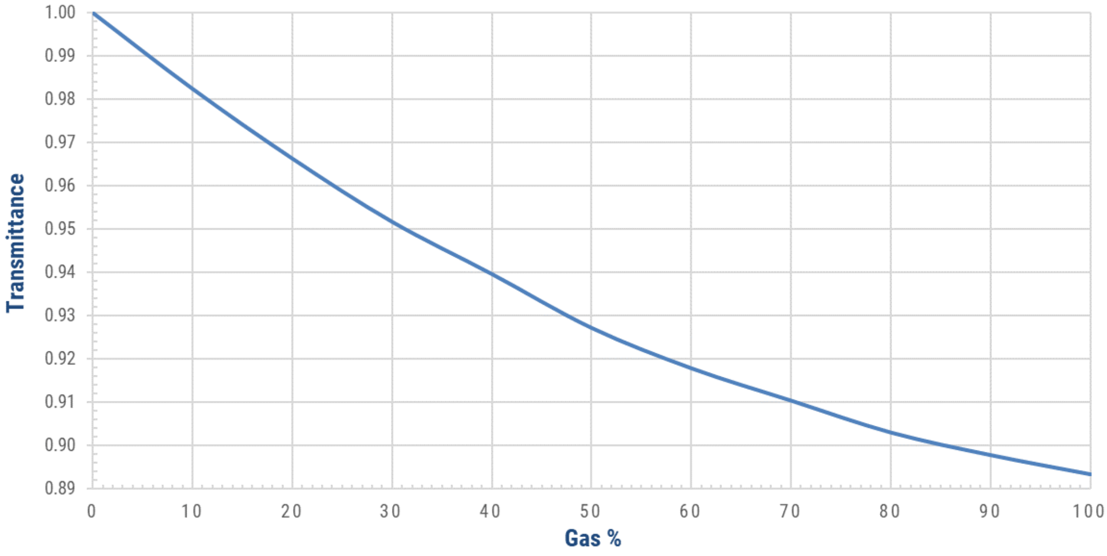


Figure 2 – Transmittance Curve

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 non-linear.

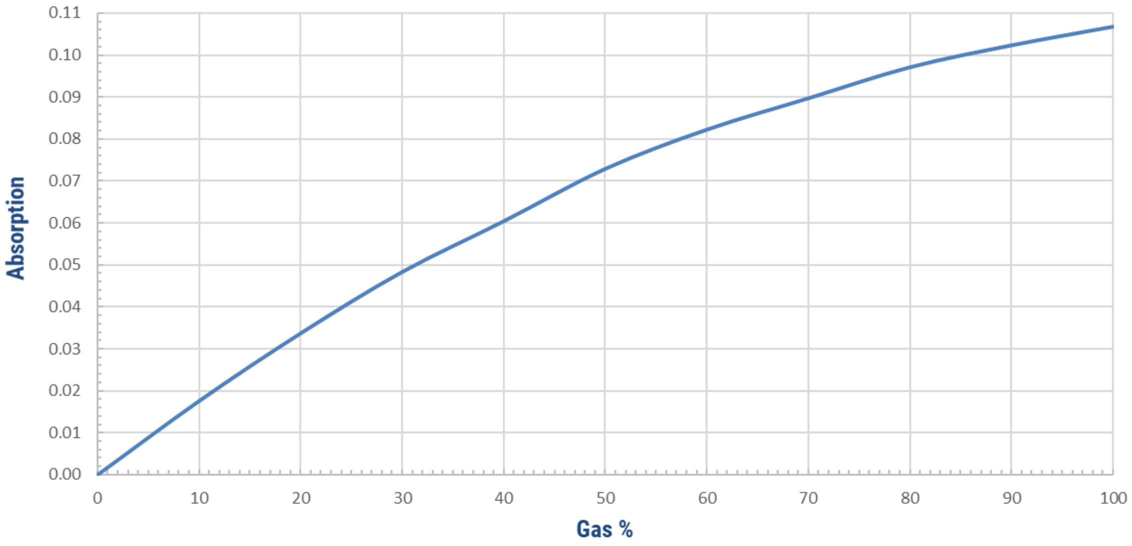


Figure 3 – Absorption Curve

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).

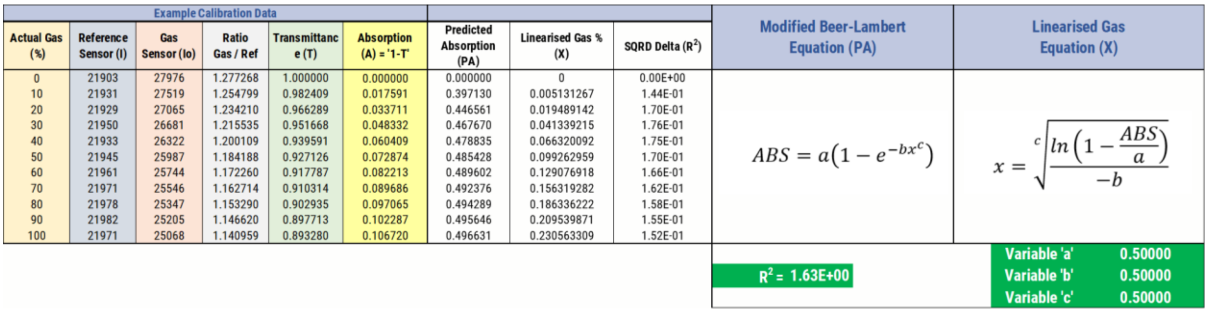
To do so, the Excel spreadsheet needs to include the **Add-ins**, and the **Solver** function.

Modified Beer-Lambert Equation (PA)	Linearised Gas Equation (X)
$ABS = a\left(1 - e^{-bx^c}\right)$	$x = \sqrt[c]{\dfrac{ln\left(1 - \dfrac{ABS}{a}\right)}{-b}}$

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^2)**: the numeric value of R^2 is used by the Excel Solver to linearise the final gas prediction.

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 Data								
Actual Gas (%)	Reference Sensor (I)	Gas Sensor (Io)	Ratio Gas / Ref	Transmittance (T)	Absorption (A) = '1-T'	Predicted Absorption (PA)	Linearised Gas % (X)	SQRD Delta (R^2)
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
50	21945	25987	1.184188	0.927126	0.072874	0.485428	0.099262959	1.70E-01
60	21961	25744	1.172260	0.917787	0.082213	0.489602	0.129076918	1.66E-01
70	21971	25546	1.162714	0.910314	0.089686	0.492376	0.156319282	1.62E-01
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

Modified Beer-Lambert Equation (PA)	Linearised Gas Equation (X)	
$ABS = a\left(1 - e^{-bx^{c}}\right)$	$x = \sqrt[c]{\frac{ln\left(1 - \frac{ABS}{a}\right)}{-b}}$	
	Variable 'a'	0.50000
$R^2 =$ 1.63E+00	Variable 'b'	0.50000
	Variable 'c'	0.50000

- Using initial values of 0.5 for each variable 'a', 'b' and 'c'.

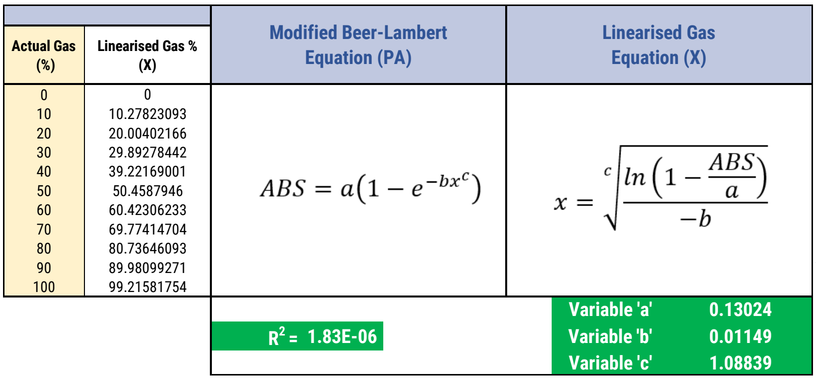
- PA and X columns are automatically populated with **estimated** values.

- Notice also that the sum of the Delta R^2 column has now been calculated as 1.63.
  This value is part of the solver function and must not 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:



Actual Gas (%)	Linearised Gas % (X)
0	0
10	10.27823093
20	20.00402166
30	29.89278442
40	39.22169001
50	50.4587946
60	60.42306233
70	69.77414704
80	80.73646093
90	89.98099271
100	99.21581754

Modified Beer-Lambert Equation (PA)	Linearised Gas Equation (X)	
$ABS = a\left(1 - e^{-bx^{c}}\right)$	$x = \sqrt[c]{\frac{ln\left(1 - \frac{ABS}{a}\right)}{-b}}$	
	Variable 'a'	0.13024
$R^2 =$ 1.83E-06	Variable 'b'	0.01149
	Variable 'c'	1.08839

Using equations **PA** and **X**, suitable values have been calculated to linearise the **expected** gas.

Plotting **Calibration Gas %** against the calculated **Linearized Gas %** shows how predictable this model is.

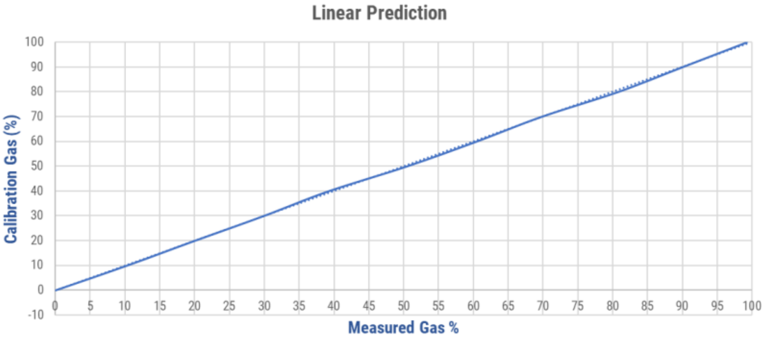


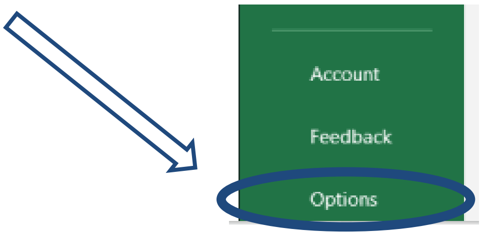
Figure 4 – Linearized Gas Prediction

3 EXCEL SPREADSHEET SOLVER ADD-IN

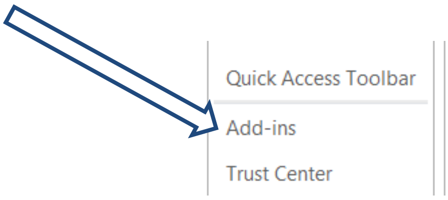
3.1 Installing the Solver

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

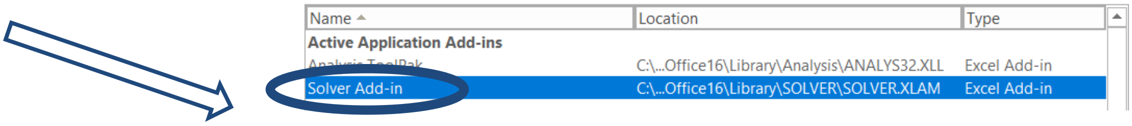
- Within Excel spreadsheet, click **File**, and then click on **Options** in the green menu.



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

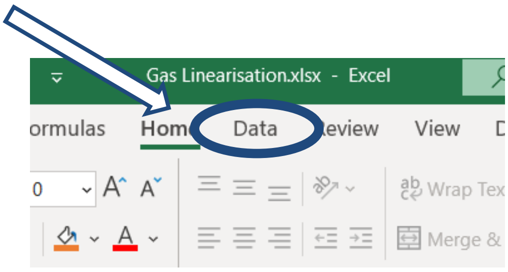


- Select **Solver Add-in**,
  Then click OK.

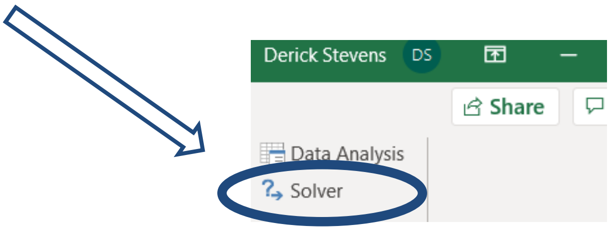


Name	Location	Type
Active Application Add-ins		
Analysis ToolPak	C:\…Office16\Library\Analysis\ANALYS32.XLL	Excel Add-in
Solver Add-in	C:\…Office16\Library\SOLVER\SOLVER.XLAM	Excel Add-in

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



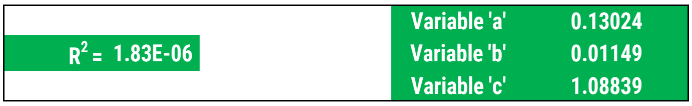
- You will now see a new function called **SOLVER,**
  this is the new function you will use to calculate the linearization variables.



3.2 Using the Solver

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

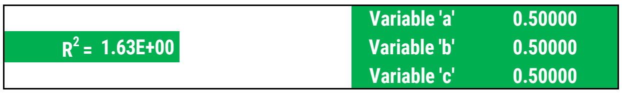
- Within the spreadsheet, identify and name four cells that will be used for the linearisation solver.
- In below example, the first cell is called R^2.
- The remaining cells are then identified as Variable 'a', Variable 'b' and Variable 'c'.



R^2 = 1.83E-06	Variable 'a'	0.13024
	Variable 'b'	0.01149
	Variable 'c'	1.08839

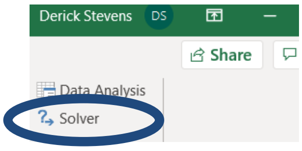
- In the example, they are cell locations $L$16 $Q$15 $Q$16 $Q$17
- Remember Cell locations as they will be required by the **Solver** function.

Initial variable conditions should be set to 0.5 and ensure R^2 value is at 1.63.



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

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

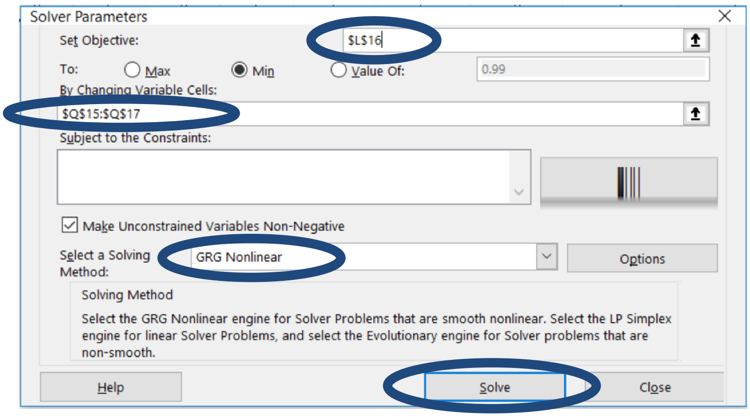


Make sure the four cells you identified in the previous step are correctly identified within the **Solver Parameters**.

The objective is identified as the result of the R^2 Cell.

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

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



Solver Parameters

Set Objective: $L$16

To: ○ Max ● Min ○ Value Of: 0.99

By Changing Variable Cells:

$Q$15:$Q$17

Subject to the Constraints:

☑ Make Unconstrained Variables Non-Negative

Select a Solving Method: GRG Nonlinear

Solving Method

Select the GRG Nonlinear engine for Solver Problems that are smooth nonlinear. Select the LP Simplex engine for linear Solver Problems, and select the Evolutionary engine for Solver problems that are non-smooth.

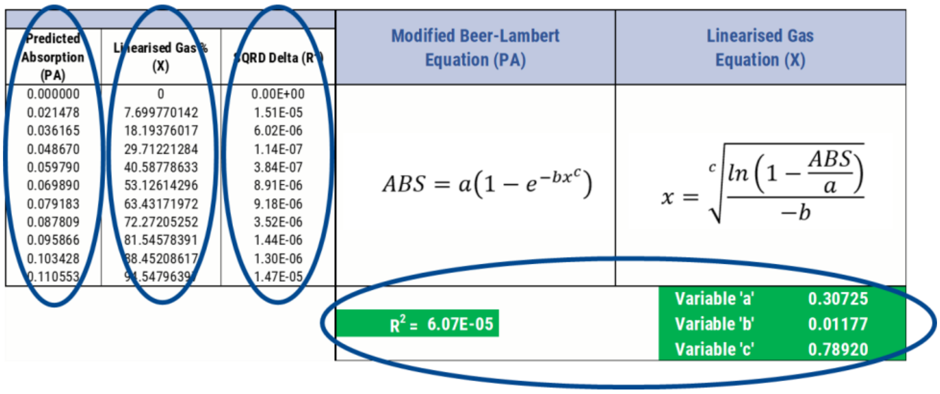
Now simply click **Solve**.

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

- the R² 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.

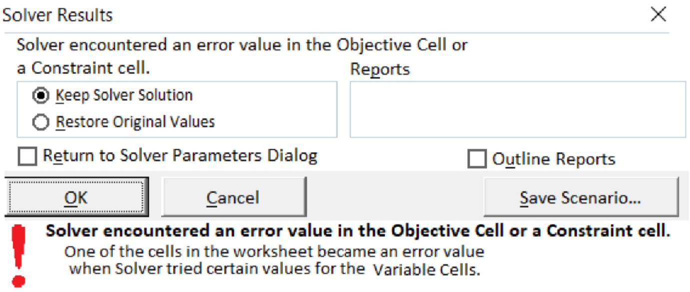


Predicted Absorption (PA)	Linearised Gas % (X)	SQRD Delta (R²)
0.000000	0	0.00E+00
0.021478	7.699770142	1.51E-05
0.036165	18.19376017	6.02E-06
0.048670	29.71221284	1.14E-07
0.059790	40.58778633	3.84E-07
0.069890	53.12614296	8.91E-06
0.079183	63.43171972	9.18E-06
0.087809	72.27205252	3.52E-06
0.095866	81.54578391	1.44E-06
0.103428	88.45208617	1.30E-06
0.110553	94.5479639	1.47E-05

Modified Beer-Lambert Equation (PA)	Linearised Gas Equation (X)
$ABS = a\left(1-e^{-bx^{c}}\right)$	$x = \sqrt[c]{\dfrac{\ln\left(1-\dfrac{ABS}{a}\right)}{-b}}$
R² = 6.07E-05	Variable 'a' 0.30725 Variable 'b' 0.01177 Variable 'c' 0.78920

Values for R², Variable ‘a’, Variable ‘b’, and Variable ‘c’ all changed.

If or when the **Solver** shows the following message just click OK.



Solver Results

Solver encountered an error value in the Objective Cell or a Constraint cell.

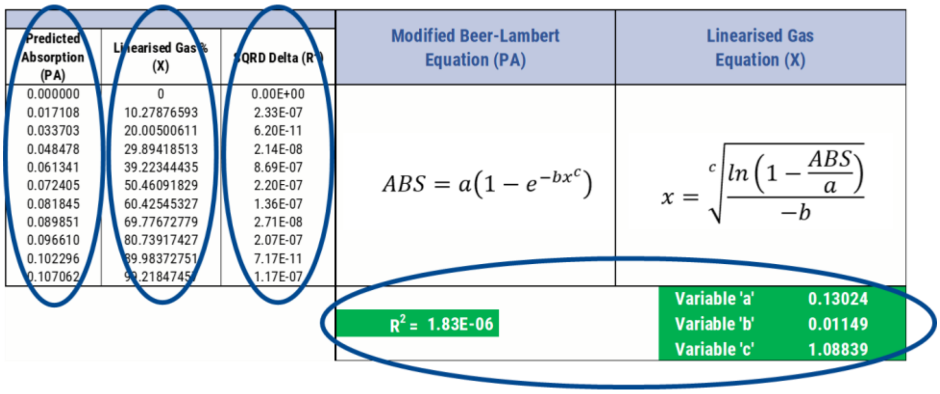
Solver encountered an error value in the Objective Cell or a Constraint cell.
One of the cells in the worksheet became an error value when Solver tried certain values for the Variable Cells.

- 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



Predicted Absorption (PA)	Linearised Gas % (X)	SQRD Delta (R²)
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
0.061341	39.22344435	8.69E-07
0.072405	50.46091829	2.20E-07
0.081845	60.42545327	1.36E-07
0.089851	69.77672779	2.71E-08
0.096610	80.73917427	2.07E-07
0.102296	89.98372751	7.17E-11
0.107062	9[illegible].2184745	1.17E-07

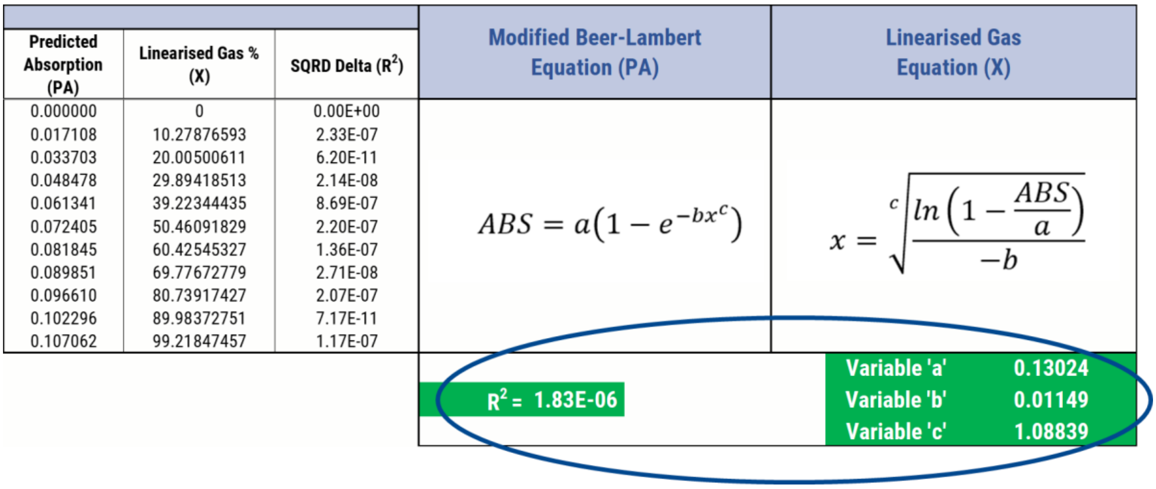
Modified Beer-Lambert Equation (PA)	Linearised Gas Equation (X)
$ABS = a\left(1-e^{-bx^{c}}\right)$	$x = \sqrt[c]{\dfrac{\ln\left(1-\dfrac{ABS}{a}\right)}{-b}}$
R² = 1.83E-06	Variable 'a' 0.13024 Variable 'b' 0.01149 Variable 'c' 1.08839

Values for R², 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^2)
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
0.061341	39.22344435	8.69E-07
0.072405	50.46091829	2.20E-07
0.081845	60.42545327	1.36E-07
0.089851	69.77672779	2.71E-08
0.096610	80.73917427	2.07E-07
0.102296	89.98372751	7.17E-11
0.107062	99.21847457	1.17E-07

Modified Beer-Lambert Equation (PA)

$$ABS = a\left(1 - e^{-bx^{c}}\right)$$

Linearised Gas Equation (X)

$$x = \sqrt[c]{\frac{ln\left(1 - \frac{ABS}{a}\right)}{-b}}$$

R^2 = 1.83E-06

Variable 'a'	**0.13024**
Variable 'b'	**0.01149**
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**.

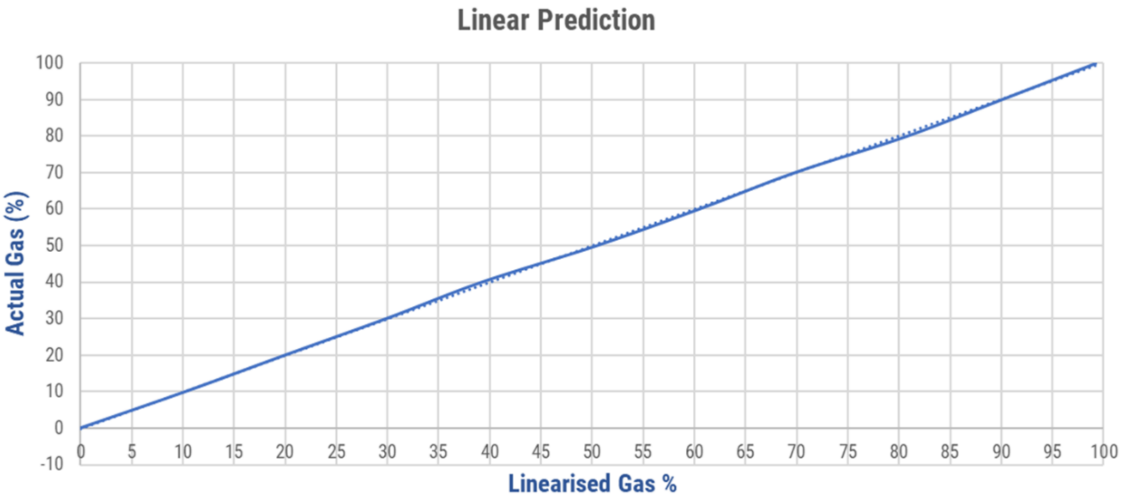


Figure 5 – Linearised Gas Prediction and Trend Line