

VPE Software: Quick Slope Alert Icon Descriptions

Abstract: This document provides a description of the alert and message icons that can appear in the SoloVPE Quick Slope module. .

Applicability: This article applies to the Quick Slope module provided with Version 2 of the SoloVPE software suite.

Symptom: Not Applicable

Cause: Not Applicable

Preface: **The Quick Slope Alert Messages in no way invalidate Quick Slope Results or indicate a problem with the Quick Slope Data. They exist merely to inform users of the actions that Quick Slope performed. When the Quick Slope results include R² values of 0.999 or greater and five or more data points, the alert messages are for reference only. If the Quick Slope results do not meet those criteria, the Alerts provide information for interpreting the results and understanding why.**

Detailed Info:

The SoloVPE Software Suite includes a software module called Quick Slope. The Quick Slope module is designed to make Slope Spectroscopy based measurements on samples. Slope measurements are made by first finding a user specified Target Absorbance value by analyzing the sample at a variety of pathlengths. The pathlength at which the Target Absorbance is found is referred to as the Threshold Pathlength. The Quick Slope algorithm will then collect a number of data points (Absorbance values at different Pathlengths) and use this dataset to perform a regression analysis to provide Slope and R² values used for quantification. Quick Slope is an autonomous module and generally runs with minimal user intervention. However, when Quick Slope encounters certain conditions it notifies the user of those conditions and the actions it took. The table below shows the indicator icon, the name and the description of the Quick Slope Indicators

Quick Slope Indicators

Icon	Name	Description
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**No Baseline
Required
Indicator**

When: Displayed following the collection of a Baseline section data which shows little or no slope.

Why: This icon is displayed to notify the user that the slope of the Baseline dataset is very small and does not appear to display pathlength dependence. This is a notification to the user that Baseline correction may not be necessary for this buffer or background media. It is strictly information and does not impact the data or results. It is intended to make the user aware in case the user wishes to investigate a non baseline corrected method.



Pathlength Shifted Down Indicator

When: Displayed following the collection of Quick Slope section data, when the Threshold Pathlength is determined to be very long.

Why: In a similar behavior to the Pathlength Shifted Up message, the Pathlength Shifted Down message is the corresponding notification that occurs when a sample is found to be very dilute. This message is displayed when the Threshold Pathlength at which the Target Absorbance level is projected to occur is above the longest pathlength measurement possible with using the current Sample Vessel in the SoloVPE. In a behavior that is consistent with the other extreme, Quick Slope collects absorbance data from the longest pathlength possible downward to show the user information that will assist them in subsequent measurements or continued data analysis. As is the case with highly concentrated samples, the software always works to show the user useful information.



Pathlength Shifted Up Indicator

When: Displayed following the collection of Quick Slope section data when the Threshold Pathlength is determined to be very short.

Why: Quick Slope first finds the Threshold Pathlength at which the Target Absorbance level is reached and then collects the specified number of data points starting at the Threshold Pathlength and moving downward to smaller pathlengths. Samples that are highly concentrated sometimes result in small Threshold Pathlengths being found. Sometimes the Threshold Pathlength is so small that given the number of data points to be collected and the pathlength step size between those data points, Quick Slope finds that negative or impossible pathlengths are required. When Quick Slope sees this condition, rather than simply generating an error for the user, Quick Slope will collect the specified number of data points but “Shifts” the pathlength range to be collected upward such that the smallest pathlength at which data is collected corresponds to the smallest pathlength the SoloVPE is capable of measuring. By doing so the longest pathlength at which data is collected no longer corresponds to the Threshold Pathlength and therefore the Absorbance values collected at the longer pathlengths will exceed the Target Absorbance level specified in the method. The reason the message is displayed is to alert the user that Quick Slope has taken an action that outside its default algorithm. This is done to make sure the user can examine the data (using Analyze of the Slope Tool) with that information in mind. A key design principle employed in the Version 2 software was that the user should always be shown information and be more knowledgeable after a run, unlike the Version 1 Quick Slope which simply generated an High Concentration error.



High Absorbance Indicator

When: Displayed following the collection of Quick Slope section data and the average absorbance of the section data exceeds the alert threshold.

Why: This icon is displayed to notify the user that the section data collected by Quick Slope displays a high average absorbance. The average absorbance of the section dataset is calculated and compared to a default threshold (System Defaults to 1.250 Abs). This alert will sometimes be displayed in conjunction with the *Pathlength Shifted Up* notification since a shift to longer pathlengths inherently results in higher absorbance values. The notification makes the user aware of conditions that may influence the measurement results. Conditions such as very high concentrations which could result cause very high absorbance values, pathlength shifts, or conditions that could be approaching the absorbance region when Beer’s Law breaks down and non-linear data could be present. These conditions will typically be confirmed with poor regression results which is easily visualized when looking at the Section plot or when the *Low R² Indicator* (See below) is turned on. The High Absorbance Indicator can also occur if there are contaminants in the optical path of the SoloVPE system which causes the system to lose light. These light losses correspond to high absorbance levels. When the anticipated concentration seems inconsistent with the absorbance level, a good troubleshooting step is to clean the optical path (e.g. Fibrette, Fibrette Coupler, Fibrette Pathway and the Delivery Fiber).

When: Displayed following the collection of Quick Slope section data and the average absorbance of the section data is below the alert threshold.

Why: This icon is displayed to notify the user that the section data collected by Quick Slope displays a low average absorbance. The average absorbance of the section dataset is calculated and compared to a default threshold (System Defaults to 0.100 Abs). This alert will sometimes be displayed in conjunction with the Pathlength Shifted Down notification since the shift to longer pathlengths will typically occur when Quick Slope cannot reach the Threshold Pathlength required to find to the Target Absorbance value. This notification makes the user aware of conditions that may influence the measurement results. Conditions such as very dilute samples, absorbance levels that approach the detection level of the device, slope resolutions that approach the limit of the device could all be influenced by very low absorbance levels. As is the case of high absorbance conditions, low absorbance conditions will also display poor regressions results and low R^2 values which may correspond to the display of the *Low R^2 Indicator* as well.



Low Absorbance Indicator

When: Displayed following the collection of Quick Slope section data and the regression statistics display R^2 results that are below a set threshold (Default of 0.9990)

Why: This icon is displayed to notify the user that the slope results have an R^2 value that is below a desired level, which by default is 0.9990. This can occur for a number of reasons including: highly concentrated (highly absorbing) samples, low concentrated (low absorbance) samples, data collected in the sample non-linear range where Beer's Law breaks down, Fibrette came out of the sample due to insufficient value in the sample vessel. There are a number of steps users can take when this occurs the simplest is to analyze the Quick Slope section data set with the Slope Tool or Analyze tools and see if removing some of the extreme data points from the analysis change the quality of the regression. There are times when the Quick Slope default of collecting ten (10) data points results in the pathlength shift and introduces some non-linearity, but fewer data points will produce consistent results. In these cases, Analyze of the Slope tool will allow users to work with the regressions to find the optimal ranges. Subsequent Quick Slope methods can then be created to target a lower Target Absorbance or specify fewer data points to be collected. There are also times with contaminants in the optical path can affect the R^2 values due to reduced transmissions. Cleaning the optical path and re-running the sample with a clean Fibrette will frequently resolve this type of issue.



Low R^2 Indicator

When: **Note* This indicator was disabled in Version 3 software.* Displayed following the collection of Quick Slope section data and the lowest data points of the section plot display a line segment with zero slope and sharply different from the line section data away from the Zero Pathlength Position.

Why: This icon is displayed to notify the user that the Fibrette in the SoloVPE may have touched the bottom of the vessel at one or more of the data points in the collected section. This indicator is displayed very infrequently because of the robust design of the SoloVPE instrument. The system looks for a specific type of discontinuity in the section data when the lower data points of the section dataset appear to flatten out. This can occur if the Fibrette tips makes contact with the bottom of the sample vessel and essentially does not move between the successive tips. If this occurs the user should check the *Zero Step Position* using the *Manual Controls*. This indicator can also turn on when very low concentrations samples are measured and the resultant slope value of the section dataset is very low to begin with. This can indicate the need to move to longer pathlength which may necessitate the larger vessel and more sample volume or the fact that the slope threshold of the device is being approached.



Possible Zero Pathlength Bump Indicator

LOW R² 999

When: **Note* This indicator was disabled in Version 3 software.* Displayed following the collection of Quick Slope section data when the highest data points of the section plot display a line segment with a discontinuous slope condition. This indicator is only active when the vessel fill feature is enabled.



Liquid Level Warning

Why: This icon is displayed to notify the user that the Fibrette may have been raised out of the sample. Quick Slope makes this determination by examining the slope of the longest pathlength data points compared to the overall dataset. If the line segment(s) at the top of the dataset appear to flatten out or become noisy, Quick Slope will display this alert making the user aware that this condition may have occurred and to examine the data more closely. It works in conjunction with the option Vessel Fill feature which asks the user to confirm the amount of sample dispensed into the vessel prior to beginning the test. Quick Slope then uses the Sample Volume and the vessel geometry to estimate the height of the sample in the vessel. It then compares that height to the pathlengths that were collected during the Quick Slope run. If the pathlengths collected approach the estimated height this warning will be displayed. *It is important to note that the feature is only based upon approximation since different samples can behave differently due to viscosity and purity and the meniscus in the vessel can vary greatly.*

Attachment: None

Document Info:

Revision History			
Rev	Date	Changes	Initials
A	2010-12-15	Initial Release	MS
01	2012-12-14	Addition of Preface segment	JF
02	2016-10-04	Addition of retired alerts and small grammatical errors	KW

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