

Stored Reference Background and the System Suitability Test for the iTX ATR Accessory

The System Suitability test has caused some confusion for our customers. This confusion is usually cleared up with a better explanation of what is actually happening during the test, especially with respect to the stored reference background. The explanation of the system suitability test is as follows...

The System Suitability (SS) was meant to give the customers a way to check the accessory performance. It also has the benefit of being able to change/modify the test criteria. For SS there are up to 5 tests that can be performed (Throughput, Contamination, Noise, X-axis accuracy, and Y-axis accuracy). The instrument performance is tested using the ValPro or Performance Verification tests

The Noise, X-axis accuracy, and Y-axis accuracy are fairly straight forward. For these tests, SS will first collect a background scan. The noise test will then collect a sample scan with no sample present (called the 100%T line) and ratio that to the background just collected. Noise is then measured in the specified region. For the X-axis accuracy and y-axis accuracy, SS will collect a scan of the 1.5 mil polystyrene standard and ratio that to the background just collected. The tests then check for proper wavenumber location and peak height for the specified peaks and compare that to the limits.

Where the confusion usually occurs is with the Throughput and Contamination tests, and these are the ones that commonly fail. This all leads back to the stored reference background. When the Throughput and Contamination tests are run, SS collects a sample scan with no sample and then ratios the scan to the **stored reference background** (not the current background). The reason for this is so that the user can determine if there has been a change in the system/accessory since the last reference was collected. For example, the IR source loses intensity over time, and if that loss is drastic enough since the last time the reference background was collected, the Throughput will fail on the low side. The opposite might happen if you install a new IR Source, where the signal intensity is now much higher and the throughput will fail on the high side. The same thing happens with the Contamination test. The current scan is ratioed to the stored reference and if there is contamination on the crystal for instance, extra peaks will show up in the spectra.

Here is the key point to remember about the stored reference background. You do not want to let it get too old, because certain tests like Throughput will eventually fail simple due to the natural loss of signal as the IR source ages. Nor do you want to simply collect a new reference background right before running SS every time, because this will defeat the purpose of the Throughput and Contamination test (they will likely never fail if you do this).

Our recommendation is to run SS on the schedule you set using the **existing** stored reference. If all the SS tests pass and the performance verification tests pass, then go ahead and collect a new reference background that will be used for the next time. That way, you are confident that the instrument and/or accessory passed the tests, but the stored reference will never get too old. If any of the SS tests fail, then you should investigate possible causes for the failures.

Each accessory might have slightly different optical characteristics based upon the mirror alignment and condition of the crystal. You should maintain separate stored backgrounds for each of the ATR accessories, because the optical differences might cause one to fail if using a stored reference background from the other. The good thing about SS, is that there is a way to do this because the SS limits and stored reference background are tied to the experiment file. So, if you have two experiment files for the golden gate accessories for example (I will call them GG1.exp and GG2.exp for simplicity), you can then run SS on Accessory 1 using GG1.exp and on Accessory 2 using GG2.exp. This way you can keep a stored reference background specific to each accessory.

You can use SS to monitor and warn you when it is due for your ATR accessory. One would leave this feature turned on and the program will warn you when the experiment file opened. You could choose to turn off the Performance Verification monitoring if you wish, but it is a good check of the instrument performance and you might want to consider continuing to run that test to validate the instruments performance. For Transmission, the PV and SS tests are essentially the same. Both are really checking the performance of the instrument. In fact, you could run the PV test with nothing in the sample compartment as well. To turn the monitoring off or to change the interval, you should choose "Configure System Status" from the View menu in OMNIC and then select the radial button for on/off. Click the Set Interval button to change the frequency of the test. There are separate options for SS and PV.

