CLAIMS

1. A computerized method for detecting and quantifying chemicals in a continuously sampled liquid or gas sample stream, comprising:

receiving, by a computing device, a sample measurement comprising a digitized spectroscopic profile;

calculating, by the computing device, a multivariate multistage background model comprising a first model that models a first time effect, and a second model that models a second time effect that is different than the first time effect;

generating, by the computing device, a background corrected sample measurement based on the sample measurement and the multivariate multistage background model; and

executing, by the computing device, a multivariate multistage library search, fault detection, and quantification algorithm to identify one or more primary chemicals in the background corrected sample measurement, the algorithm comprising:

identifying one or more candidate chemicals in the background corrected sample measurement based on a multivariate statistical process control in comparison of the background corrected sample measurement to a spectral reference library; and

performing at least one of (i) identifying a first primary chemical based on a focused chemical evaluation of the one or more candidate chemicals or (ii) quantifying the first primary chemical based on the focused chemical evaluation of the one or more candidate chemicals.

2. The method of claim 1, wherein identifying the first primary chemical comprises determining there are zero primary chemicals.

3. The method of claim 1, whercin calculating comprises updating the multivariate multistage background model.

4. The method of claim 1, wherein the multivariate multistage library search, fault detection, and quantification algorithm further comprises:

calculating a residual profile by subtracting the first primary chemical from the background corrected sample measurement;

quantifying content by estimating the first primary chemical concentration from the background corrected sample measurement;

identifying a second set of one or more candidate chemicals in the residual profile based on a comparison of the residual profile to the spectral reference library; and

identifying a second primary chemical based on a focused chemical evaluation of the second set of one or more candidate chemicals.

5. The method of claim 1, further comprising:

determining the sample measurement is suitable for inclusion into the multivariate multistage background model; and

updating the multivariate multistage background model based on the sample measurement.

6. The method of claim 5, further comprising filtering the sample measurement through a data buffer to prevent contamination resulting from slow chemical data poisoning in the sample stream.

7. The method of claim 6, wherein a size of the data buffer is determined based on a data poisoning rate value.

8. The method of claim 5, further comprising reducing an influence of one or more interference chemicals in the sample measurement based on a mask function.

9. The method of claim 8, further comprising:

identifying one or more chemical interferents; and

updating the mask function based on one or more identified chemical interferents.

10. The method of claim 5, further comprising defining one or more update conditions, comprising:

updating at least one of (i) the multivariate multistage background model or (ii) the multivariate multistage library search, fault detection, and quantification model, if zero chemical compounds are detected in the sample measurement;

updating at least one of (i) the multivariate multistage background model or (ii) the multivariate multistage library search, fault detection, and quantification model, if zero interest chemical compounds are detected in the sample measurement;

updating at least one of (i) the multivariate multistage background model or (ii) the multivariate multistage library search, fault detection, and quantification model, if there is no alarm of any interest chemical compounds in the sample measurement; or

not updating at least one of (i) the multivariate multistage model or (ii) the multivariate multistage library search, fault detection, and quantification model.

11. A system for detecting and quantifying chemicals in a continuously sampled liquid or gas sample stream, comprising:

a data acquisition module configured to receive a sample measurement comprising a digitized spectroscopic profile;

a multivariate multistage background module in communication with the data acquisition module configured to:

calculate a multivariate multistage background model comprising a first model that models a first time effect, and a second model that models a second time effect that is different than the first time effect;

generate a background corrected sample measurement based on the sample measurement and the multivariate multistage background model; and

a multivariate multistage library search, fault detection, and quantification module in communication with the data acquisition module and the multivariate multistage background module configured to execute a multivariate multistage library search, fault detection, and quantification algorithm to identify one or more primary chemicals in the background corrected sample measurement, configured to:

identify one or more candidate chemicals in the background corrected sample measurement based on a comparison of the background corrected sample measurement to a spectral reference library; and

perform at least one of (i) identifying a first primary chemical based on a focused chemical evaluation of the one or more candidate chemicals or (ii)

quantifying the first primary chemical based on the focused chemical evaluation of the one or more candidate chemicals.

12. A computerized method for detecting and quantifying chemicals in a continuously sampled liquid or gas sample stream, comprising:

repeatedly executing, by the computing device, a multivariate multistage library search, fault detection, and quantification algorithm to identify one or more primary chemicals in a sample measurement when a candidate chemical of the sample measurement is greater than a predetermined threshold, the sample measurement comprising a digitized spectroscopic profile, comprising:

identifying one or more candidate chemicals in a sample measurement based on a comparison of the sample measurement to a spectral reference library;

identifying a primary chemical of the one or more primary chemicals from the one or more candidate chemicals based on a focused chemical evaluation of the one or more candidate chemicals; and

determining whether any of the remaining one or more candidate chemicals are greater than the predetermined threshold.

13. The method of claim 12, wherein identifying a primary chemical comprises determining there are zero primary chemicals.

14. The method of claim 12, wherein the sample measurement is a background corrected sample measurement calculated based on a multivariate multistage background model.

15. The method of claim 12, wherein the one or more candidate chemicals are identified based on a matrix-based simultaneous comparison comprising a least squares regression.

16. The method of claim 15, wherein the least squares regression comprises classical least squares, partial least squares, inverse least squares, or any combination thereof.

17. The method of claim 12, further comprising:

identifying the one or more candidate chemicals based on a multivariate regression; and

identifying the primary chemical of the one or more primary chemicals based on a least squares regression.

18. The method of claim 12, wherein identifying the primary chemical of the one or more primary chemicals comprises:

calculating a root mean square of a digitized spectrum of each of the one or more candidate chemicals;

calculating a concentration of each of the one or more candidate chemicals;

calculating a *t*-statistic of the digitized spectra of each of the one or more candidate chemicals, wherein the *t*-statistic is based on a variance of the associated candidate chemical of the one or more candidate chemicals; and

identifying the first primary chemical primary chemical from the one or more candidate chemicals, wherein the first primary chemical comprises a lowest root mean square and highest *t*-statistic of the one or more candidate chemicals.

19. The method of claim 12, wherein the spectral reference library is constant, the spectral reference library is dynamically updated to include or exclude spectra, or both.

20. The method of claim 12, wherein the spectral reference library is dynamically augmented with a multivariate noise model.

21. A system for detecting and quantifying chemicals in a continuously sampled liquid or gas sample stream, comprising:

a multivariate multistage library search, fault detection, and quantification module in communication with the data acquisition module and the multivariate multistage background module configured to repeatedly execute a multivariate multistage library search, fault detection, and quantification algorithm to identify one or more primary chemicals in a sample measurement when a candidate chemical of the sample measurement is greater than a predetermined threshold, the sample measurement comprising a digitized spectroscopic profile, comprising:

a fault detection module configured to identify one or more candidate chemicals in a sample measurement based on a comparison of the sample measurement to a spectral reference library; and

a library search module in communication with the fault detection module configured to:

identify a first primary chemical from the one or more candidate chemicals based on a focused chemical evaluation of the one or more candidate chemicals; and

determine whether any of the remaining one or more candidate chemicals are greater than the predetermined threshold.

22. A computerized method for detecting and quantifying chemicals in a continuously sampled liquid or gas sample stream, comprising:

receiving, by a computing device, a sample measurement comprising a digitized spectroscopic profile;

calculating, by the computing device, a multivariate multistage background model comprising at least a first model that models a first time effect and a second model that models a second time effect that is different than the first time effect;

generating, by the computing device, a background corrected sample measurement based on the sample measurement and the multivariate multistage background model;

determining, by the computing device, the sample measurement is suitable for inclusion as an update to the multivariate multistage background model; and

updating, by the computing device, the multivariate multistage background model based on the sample measurement.

23. The method of claim 22, where the first model of the multivariate multistage background model comprises an evolving background model.

24. The method of claim 23, further comprising:

initiating a background spectrum of the evolving background model in a time domain, a frequency domain, or both, based on an exponentially weighted moving average; and

updating the background spectrum based on the exponentially weighted moving average.

25. The method of claim 22, where the second model of the multivariate multistage background algorithm comprises a multivariate noise model.

26. The method of claim 25, further comprising:

filtering the multivariate noise model based on the first model; and

correcting a remaining spectral variation of the multivariate noise model based on a multivariate approach comprising principal components analysis, independent components analysis, multivariate curve resolution, partial least squares, weighted least squares, total least squares, continuum regression, ridge regression, or any combination thereof.

27. The method of claim 26, further comprising updating the multivariate noise model based on an exponentially weighted multivariate approach to minimize a residual profile of the corrected remaining spectral variation, wherein the exponentially weighted multivariate approach comprises exponentially weighted moving principal components analysis, exponentially weighted moving independent components analysis, exponentially weighted moving multivariate curve resolution, exponentially weighted moving partial least squares, exponentially weighted moving total least squares, exponentially weighted moving continuum regression, exponentially weighted moving ridge regression, or any combination thereof.

28. A system for detecting and quantifying chemicals in a continuously sampled liquid or gas sample stream, comprising:

a data acquisition module configured to receive a sample measurement comprising a digitized spectroscopic profile;

a multivariate multistage background module in communication with the data acquisition module configured to:

calculate a multivariate multistage background model comprising at least a first model that models a first time effect and a second model that models a second time effect that is different than the first time effect;

generate a background corrected sample measurement based on the sample measurement and the multivariate multistage background model; and

update the multivariate multistage background model based on the sample measurement; and

a data quality diagnostic module in communication with the multivariate multistage background module configured to determine the sample measurement is suitable for inclusion as an update to the multivariate multistage background model.

29. A computer program product, tangibly embodied in a computer readable storage medium, the computer program product including instructions being operable to cause a data processing apparatus to:

receive a sample measurement comprising a digitized spectroscopic profile;

calculate a multivariate multistage background model comprising a first model that models a first time effect, and a second model that models a second time effect that is different than the first time effect;

generate a background corrected sample measurement based on the sample measurement and the multivariate multistage background model; and

execute a multivariate multistage library search, fault detection, and quantification algorithm to identify one or more primary chemicals in the background corrected sample measurement, the algorithm being configured to:

identify one or more candidate chemicals in the background corrected sample measurement based on a multivariate statistical process control in comparison of the background corrected sample measurement to a spectral reference library; and

identify a first primary chemical based on a focused chemical evaluation of the one or more candidate chemicals.

30. A computer program product, tangibly embodied in a computer readable storage medium, the computer program product including instructions being operable to cause a data processing apparatus to:

repeatedly execute a multivariate multistage library search, fault detection, and quantification algorithm to identify one or more primary chemicals in a sample measurement when a candidate chemical of the sample measurement is greater than a predetermined threshold, the sample measurement comprising a digitized spectroscopic profile, the algorithm being configured to:

identify one or more candidate chemicals in a sample measurement based on a comparison of the sample measurement to a spectral reference library;

identify a primary chemical of the one or more primary chemicals from the one or more candidate chemicals based on a focused chemical evaluation of the one or more candidate chemicals; and

determine whether any of the remaining one or more candidate chemicals are greater than the predetermined threshold.

31. A computer program product, tangibly embodied in a computer readable storage medium, the computer program product including instructions being operable to cause a data processing apparatus to:

receive a sample measurement comprising a digitized spectroscopic profile;

calculate a multivariate multistage background model comprising at least a first model that models a first time effect and a second model that models a second time effect that is different than the first time effect;

generate a background corrected sample measurement based on the sample measurement and the multivariate multistage background model;

determine the sample measurement is suitable for inclusion as an update to the multivariate multistage background model; and

update the multivariate multistage background model based on the sample measurement.

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1. A computerized method for detecting and quantifying chemicals in a continuously sampled liquid or gas sample stream, comprising:

receiving, by a computing device, a sample measurement comprising a digitized spectroscopic profile;

calculating, by the computing device, a multivariate multistage background model comprising a first model that models a first time effect, a second model that models a second time effect that is different than the first time effect, or both;

generating, by the computing device, a background corrected sample measurement based on the sample measurement and the multivariate multistage background model; and

executing, by the computing device, a multivariate multistage library search, fault detection, and quantification algorithm to identify one or more primary chemicals in the background corrected sample measurement, the algorithm comprising:

identifying one or more candidate chemicals in the background corrected sample measurement based on a multivariate statistical process control in comparison of the background corrected sample measurement to a spectral reference library;

performing at least one of (i) identifying a first primary chemical based on a focused chemical evaluation of the one or more candidate chemicals or (ii) quantifying the first primary chemical based on the focused chemical evaluation of the one or more candidate chemicals;

calculating a residual profile by subtracting the first primary chemical from the background corrected sample measurement; and

identifying a second set of one or more candidate chemicals in the residual profile based on a comparison of the residual profile to the spectral reference library.

2. The method of claim 1, wherein identifying the first primary chemical comprises determining there are zero primary chemicals.

3. The method of claim 1, wherein calculating comprises updating the multivariate multistage background model.

4. The method of claim 1, wherein the multivariate multistage library search, fault detection, and quantification algorithm further comprises:

quantifying content by estimating the first primary chemical concentration from the background corrected sample measurement; and

identifying a second primary chemical based on a focused chemical evaluation of the second set of one or more candidate chemicals.

5. The method of claim 1, further comprising:

determining the sample measurement is suitable for inclusion into the multivariate multistage background model; and

updating the multivariate multistage background model based on the sample measurement.

6. The method of claim 5, further comprising filtering the sample measurement through a data buffer to prevent contamination resulting from slow chemical data poisoning in the sample stream.

7. The method of claim 6, wherein a size of the data buffer is determined based on a data poisoning rate value.

8. The method of claim 5, further comprising reducing an influence of one or more interference chemicals in the sample measurement based on a mask function.

9. The method of claim 8, further comprising:

identifying one or more chemical interferents; and

updating the mask function based on one or more identified chemical interferents.

10. The method of claim 5, further comprising defining one or more update conditions, comprising:

updating at least one of (i) the multivariate multistage background model or (ii) the multivariate multistage library search, fault detection, and quantification model, if zero chemical compounds are detected in the sample measurement;

updating at least one of (i) the multivariate multistage background model or (ii) the multivariate multistage library search, fault detection, and quantification model, if zero interest chemical compounds are detected in the sample measurement;

updating at least one of (i) the multivariate multistage background model or (ii) the multivariate multistage library search, fault detection, and quantification model, if there is no alarm of any interest chemical compounds in the sample measurement; or

not updating at least one of (i) the multivariate multistage model or (ii) the multivariate multistage library search, fault detection, and quantification model.

11. A system for detecting and quantifying chemicals in a continuously sampled liquid or gas sample stream, comprising:

a data acquisition module configured to receive a sample measurement comprising a digitized spectroscopic profile;

a multivariate multistage background module in communication with the data acquisition module configured to:

calculate a multivariate multistage background model comprising a first model that models a first time effect, a second model that models a second time effect that is different than the first time effect, or both;

generate a background corrected sample measurement based on the sample measurement and the multivariate multistage background model; and

a multivariate multistage library search, fault detection, and quantification module in communication with the data acquisition module and the multivariate multistage background module configured to execute a multivariate multistage library search, fault detection, and quantification algorithm to identify one or more primary chemicals in the background corrected sample measurement, configured to:

identify one or more candidate chemicals in the background corrected sample measurement based on a comparison of the background corrected sample measurement to a spectral reference library;

perform at least one of (i) identifying a first primary chemical based on a focused chemical evaluation of the one or more candidate chemicals or (ii) quantifying the first primary chemical based on the focused chemical evaluation of the one or more candidate chemicals;

calculate a residual profile by subtracting the first primary chemical from the background corrected sample measurement; and

identify a second set of one or more candidate chemicals in the residual profile based on a comparison of the residual profile to the spectral reference library.

12. A non-transitory computer readable medium containing computer instructions stored therein for causing a data processing apparatus to:

receive a sample measurement comprising a digitized spectroscopic profile;

calculate a multivariate multistage background model comprising a first model that models a first time effect, a second model that models a second time effect that is different than the first time effect, or both;

generate a background corrected sample measurement based on the sample measurement and the multivariate multistage background model; and

execute a multivariate multistage library search, fault detection, and quantification algorithm to identify one or more primary chemicals in the background corrected sample measurement, the algorithm being configured to:

identify one or more candidate chemicals in the background corrected sample measurement based on a multivariate statistical process control in comparison of the background corrected sample measurement to a spectral reference library;

identify a first primary chemical based on a focused chemical evaluation of the one or more candidate chemicals;

calculate a residual profile by subtracting the first primary chemical from the background corrected sample measurement; and

identify a second set of one or more candidate chemicals in the residual profile based on a comparison of the residual profile to the spectral reference library.