Application Note

May 2026

Keywords or phrases:
Direct transition analysis, chromatography, multivariate data analysis, process monitoring

Multivariate Direct Transition Analysis in Chromatography Using SIMCA® and SIMCA®-online

Amin Ganjian[1], Scott Carpenter[2], Gregory Casee[2]
[1] Sartorius Canada Inc. 1173 North Service Road West, Unit D-4, Oakville, Ontario L6M 2V9, Canada
[2] Sartorius Stedim North America Inc. 545-1 Johnson Avenue, Bohemia, NY 11716, USA

Contact: amin.ganjian@sartorius.com

Abstract

Column chromatography is a crucial step in the separation and purification of biopharmaceutical products. To ensure consistent product quality across batches, it is essential to monitor column performance under varying operational conditions. The traditional salt-plug test, commonly used for batch-to-batch column assessment, is often too impractical for routine operations. Moment analysis is an alternative method that involves analyzing transition curves during phase changes; however, it has limitations, particularly for multi-column chromatography.

Direct transition analysis provides a robust, sensitive, and straightforward approach for process monitoring through operational transition analysis. This application note reviews the benefits of implementing direct transition analysis for operational assessment, illustrated by four case studies using manufacturing-scale chromatography data.

Introduction

Chromatography column monitoring

Salt-plug test

Consistent high performance of column chromatography in downstream biopharmaceutical production is key to consistent product quality.[1] One of the early methods to assess column consistency is called the salt-plug (pulsed-input) test, where a chemical tracer is injected into the column to observe a bell-shaped curve (Gaussian distribution curve) formed at the column outlet.[2]

Height equivalent of a theoretical plate (HETP) and asymmetry factor (Af) are the two most common metrics extracted from the shape of the curve.[3-5] Batch-to-batch assessment using the salt-plug test involves comparing the bell-shaped curve, along with HETP and Af, for the monitoring batch against those of referenced "golden" batches. One limitation of the salt-plug test is that it is labor-intensive, as it requires auxiliary equipment for chemical tracer injection and introduces additional procedures that are not part of routine product purification. HETP and Af also have limited sensitivity and require a degree of subjectivity when establishing the mathematical approach (peak and baseline identification).[6]

Moment analysis

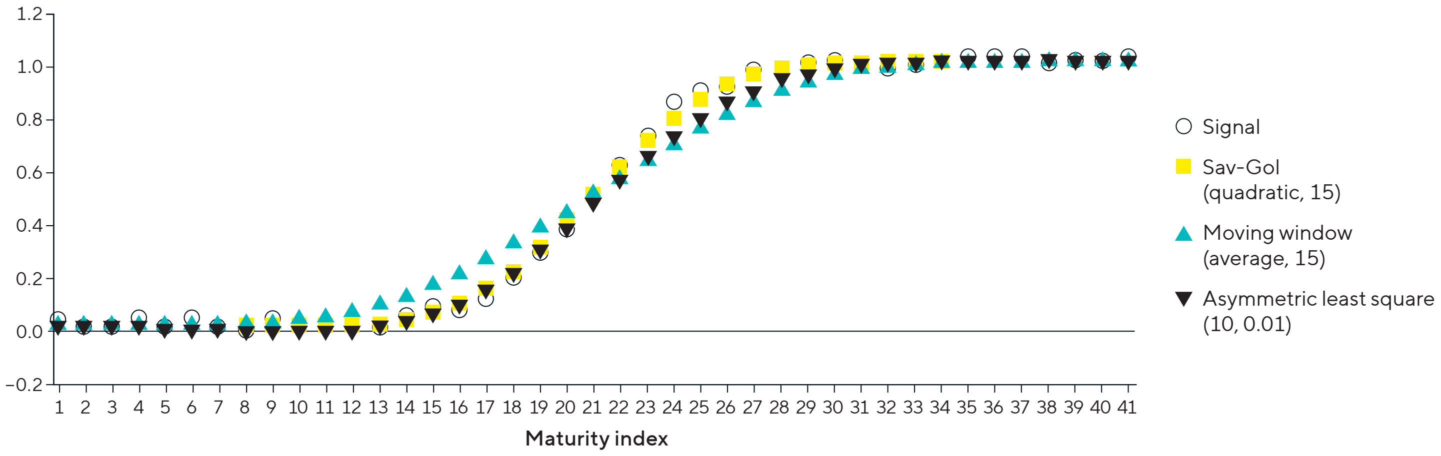
To simplify operational procedures that include batch-to-batch column performance assessment, moment analysis (MA) can be performed by extracting information from the bell-shaped curve of the salt-plug test.[7,8] In this approach, the first derivative of a detection signal resulting from a buffer change is used for column assessment. Since buffer change is part of the production operation recipe, no additional procedures are required to perform the test, no trace element is injected into the column, and no auxiliary equipment is required. The first derivative of a transition curve is typically bell-shaped, enabling the extraction of HETP and Af with subjective mathematical considerations.[9]

Although MA simplifies operations, it is associated with increased analytical effort of estimating the derivative, which typically requires extensive data treatment, mathematical approximation, and subjectivity introduced by the method developer.

Data treatment in MA

To estimate the first derivative, the transition curve is first approximated by a smoothing algorithm. The selection of the smoothing method affects not only the approximation of the transition curve, but also the calculation of the first derivative required for HETP and Af determination. This level of subjectivity hinders standardization and challenges its use as a definitive method for assessing batch-to-batch column chromatography. Figure 1 illustrates the variations in approximation when three common smoothing algorithms are applied to a transition profile.[10-12]

Figure 1: Approximation of a transition profile (signal) by three smoothing filters: Savitzky-Golay (Sav-Gol), moving window average, and asymmetric least squares



Methods

Direct transition analysis

Method description
To leverage the benefits of transition analysis while addressing the limitations of MA, direct transition analysis (DTA) was developed within the biopharmaceutical industry.[6] In DTA, analytical metrics are directly derived from a transition profile with minimal signal processing. In this approach, 13 threshold levels of 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.5, 0.7, 0.75, 0.8, 0.85, 0.9, and 0.95 are identified for a transition profile normalized between 0 (minimum) and 1 (maximum).

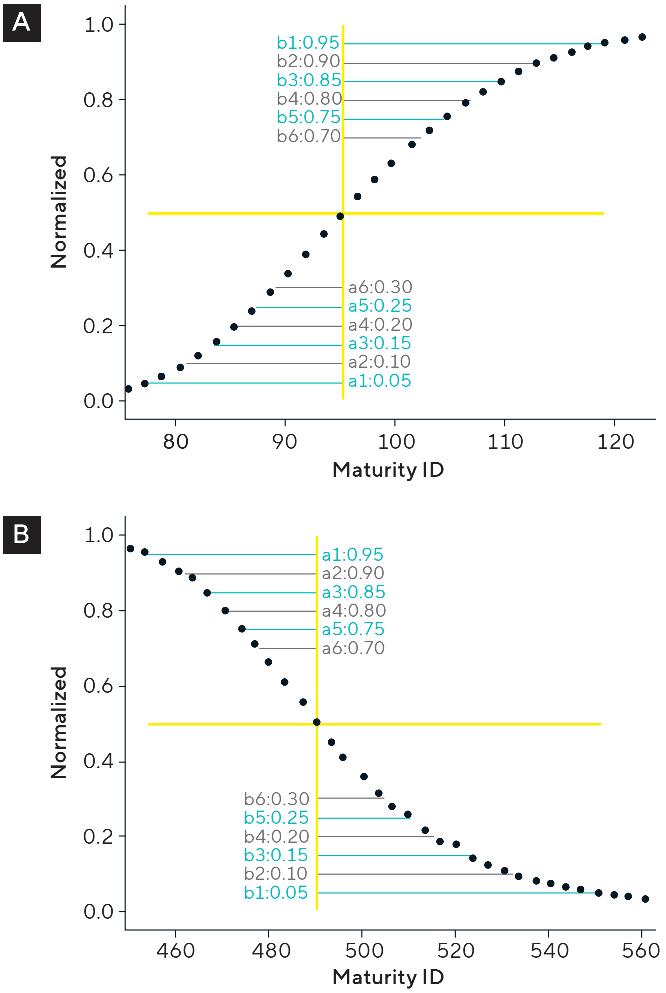
As depicted in Figure 2, the linear approximation of the two available data points nearest to each threshold is used. The CenterPoint of 0.5 is set as the reference to calculate 12 DTA elements as the absolute difference between the CenterPoint and the thresholds (a_i leading elements and b_i tailing elements).

DTA metrics are defined as b_i/a_i ratios, DirectAf is defined as $\sum_{i=1}^{6}(\frac{b_i}{a_i})$ and TransWidth is defined as (a_1+b_1).

Description of the transition types
There are two general types of transition profiles: (1) positive-going transitions, where the detection signal increases over the course of a transition, and (2) negative-going transitions, where the detection signal decreases from the head to the tail of a transition.

Figure 2A demonstrates an example of a positive-going transition, while Figure 2B depicts a negative-going transition along with DTA thresholds, elements, and metrics calculated for each case. DTA breakthrough is defined as the point where the transition profile meets the first threshold of 0.05 for positive-going and 0.95 for negative-going transition profiles.

Figure 2: An example of a positive-going transition profile **(A)** and a negative-going transition profile **(B)** depicting DTA thresholds, elements, and metrics



A

DTA Thresholds (Maturity ID)
95% = 118.35
90% = 112.79
85% = 109.38
80% = 106.56
75% = 104.20
70% = 102.01
50% = 95.115
30% = 88.849
25% = 87.188
20% = 85.358
15% = 83.265
10% = 80.899
05% = 77.501

DTA elements
b1 = 23.238
b2 = 17.683
b3 = 14.266
b4 = 11.451
b5 = 9.0853
b6 = 6.9006
a6 = 6.2663
a5 = 7.9273
a4 = 9.7569
a3 = 11.850
a2 = 14.216
a1 = 17.614

DTA metrics
b1/a1 = 1.3193
b2/a2 = 1.2438
b3/a3 = 1.2038
b4/a4 = 1.1736
b5/a5 = 1.1460
b6/a6 = 1.1012
DirectAf
AVG(b/a) = 1.197
TransWidth
a1 + b1 = 40.852
CenterPoint
50% = 95.115
Breakthrough
5% = 77.501

B

DTA Thresholds (Maturity ID)
95% = 453.76
90% = 461.32
85% = 466.09
80% = 470.13
75% = 473.82
70% = 477.37
50% = 489.95
30% = 504.31
25% = 510.24
20% = 514.96
15% = 522.52
10% = 532.15
05% = 550.88

DTA elements
a1 = 36.181
a2 = 28.629
a3 = 23.857
a4 = 19.815
a5 = 16.123
a6 = 12.581
b6 = 14.363
b5 = 20.288
b4 = 25.013
b3 = 32.575
b2 = 42.202
b1 = 60.930

DTA metrics
b1/a1 = 1.6840
b2/a2 = 1.4740
b3/a3 = 1.3654
b4/a4 = 1.2623
b5/a5 = 1.2583
b6/a6 = 1.1416
DirectAf
AVG(b/a) = 1.364
TransWidth
a1 + b1 = 97.112
CenterPoint
50% = 489.95
Breakthrough
95% = 453.76

Results

Addressing limitations observed in MA

DTA does not require the estimation of a derivative profile and is independent of subjective approximations introduced by a method developer.

Unlike moment analysis, DTA metrics are agnostic to the buffer change timestamp because the CenterPoint is set as a reference for calculations. This is a considerable advantage of DTA over MA, as the primary objective of real-world application of the monitoring methods is to provide a tool capable of defining standardized criteria for batch-to-batch comparison. These criteria can be used to establish proper statistical monitoring schemes, rather than focusing on the absolute values in each run.

Multivariate data analysis for DTA

DTA thresholds, elements, and metrics provide over twenty-five criteria suitable for batch-to-batch performance assessment of a chromatography column. The multivariate nature of the DTA-derived criteria necessitates the application of multivariate data analysis (MVDA) methods, such as principal component analysis (PCA), for unsupervised dimension reduction.[13]

MVDA orthogonal projections to latent structures (OPLS®) is also a suitable tool for regressing DTA components against process quality or quantity metrics.[14-16] In the presence of different operational packing methods, levels of process efficiency (low, medium, or high), and product release test categories (pass or fail), OPLS® discriminant analysis (OPLS®-DA) can maximize the covariance in DTA components to enable class difference segregation and potentially prediction of the class.[17] In addition to the representation of each batch process by dimensionally distilled score values of an MVDA model, DModX (distance to the model for X-data) is available to better enable identification of process abnormalities as outliers.[18]

MVDA-DTA by SIMCA® and SIMCA®-online

SIMCA® and SIMCA®-online (Sartorius) are two software solutions that enable MVDA model development and execution for offline historical data analysis and online process monitoring, respectively.[17,18] To enable the execution of MVDA on DTA components for online batch-to-batch chromatography process assessment, a software module plug-in can be embedded in both SIMCA® and SIMCA®-online called the DTA SIMCA® Extension. Once an MVDA-DTA model is developed for process data in SIMCA®, it can be seamlessly transferred to SIMCA®-online for monitoring the production skid. Upon completion of a transition profile in a chromatography process monitored by SIMCA®-online, DTA metrics are extracted and assessed using a multivariate statistical process control scheme.

MVDA-DTA model creation in SIMCA®

The DTA SIMCA® Extension is executable in batch level mode (BLM), where data related to each batch is captured in one vector. For each chromatography batch, at the end of a transition phase, a BLM model developed in SIMCA® would be executable in both SIMCA® and SIMCA®-online. As mentioned, the BLM multivariate model can be of any type (PCA, OPLS®, OPLS®-DA) depending on process data availability and the analytical scheme considered for monitoring. DTA variables calculated by the module in BLM would be used to build an MVDA model in BLM.

The DTA SIMCA® Extension was developed to capture the single process parameter that presents transition by a detection signal (i.e., conductivity or UV). The process maturity index (which monotonically increases to capture process progression) is generally the cumulative volume (CV) of the moving liquid phase in column chromatography.

MVDA-DTA model execution in SIMCA® and SIMCA®-online

Upon exposure of a new transition profile to the model built using DTA variables generated by the DTA SIMCA® Extension, DTA variables are automatically calculated and summarized by the MVDA model in SIMCA® or SIMCA®-online. Based on historical data analysis of a process in SIMCA®, suitable univariate and multivariate process control and monitoring schemes can be defined and applied in SIMCA®-online for batch-to-batch performance assessment of a chromatography column.

Case Studies

MVDA-DTA case studies using biopharmaceutical manufacturing data

An evaluation of the chromatography column monitoring method for MVDA-DTA-based performance assessment was conducted using process data from four major biopharmaceutical manufacturing companies. The list includes AstraZeneca, Lilly, Lonza, and Takeda.

In the first case study, the identification of normal versus abnormal transitions by MVDA-DTA is demonstrated. A second MVDA-DTA model is constructed using acceptable transitions and subsequently tested by assessing all data using the SIMCA® outlier detection tool.

In the second case study, the classification provided for the batch processes was based on product quality regardless of transitions observed in the chromatography process. The study confirms the ability of MVDA-DTA to distinguish between acceptable and undesirable batches by analyzing chromatography transition profiles. A second model is built using transitions from acceptable batches to demonstrate that DModX could identify undesirable batches using the transition profiles.

In the third case study, MVDA-DTA demonstrates an effective monitoring scheme for resin usage and packing method based on conductivity transitions in the process equilibration phase.

In the fourth case study, MVDA-DTA can detect a process changepoint in batch-to-batch assessment, confirming improved process robustness following the process change point.

Case Study 1: Differentiating normal and abnormal transitions
As a proof of concept, a dataset containing 17 transition profiles of post-column conductivity (mS/cm) over CV (L) in the wash phase for manufacturing-scale column chromatography was provided. The process subject matter expert (SME) identified 12 transitions as normal (acceptable) and five as abnormal (undesirable) transitions (Figure 3).

Transition profiles were transferred to SIMCA®, the DTA SIMCA® Extension was executed in BLM, and a PCA model was fitted using the DTA variables generated by the module.

Figure 3: Profiles of five undesirable transitions (U) in black and twelve acceptable transitions (A) in yellow

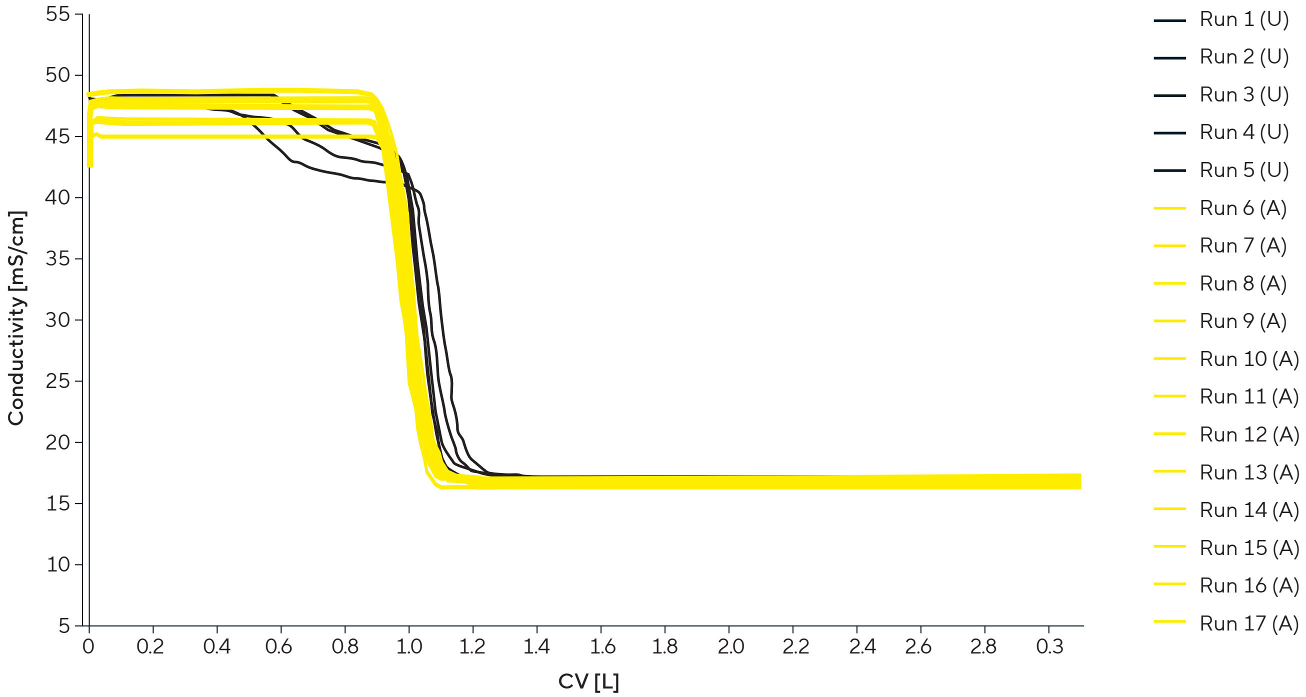


Figure 4 demonstrates that the scores of the first principal component (t[1]) could segregate acceptable and undesirable transitions identified by the process SME. The sign of the first principal component score calculated for each profile indicates the group type of the transition. For this model, abnormal, undesirable transitions have positive signs, and normal, acceptable transitions have negative signs.

SIMCA® offers "drill-down" capabilities to assess the contributions of variables to the differences between groups of selected data. A score contribution close to zero indicates that the variable makes an insignificant contribution to the difference between the selected groups. On the other hand, high score contributions indicate variables that have a more significant effect on the group difference.

As depicted in Figure 5, acceptable and undesirable transitions are captured by multiple DTA components. DTA element a1 has the highest negative contribution (undesirable black group a1 values are substantially higher than acceptable yellow group a1 values in Figure 6). Conversely, the DTA 95% threshold has the highest positive contribution (undesirable black group 95% thresholds are substantially lower than acceptable yellow group 95% thresholds in Figure 6).

Figure 4: Scores of the first principal component for the PCA model fitted on DTA components

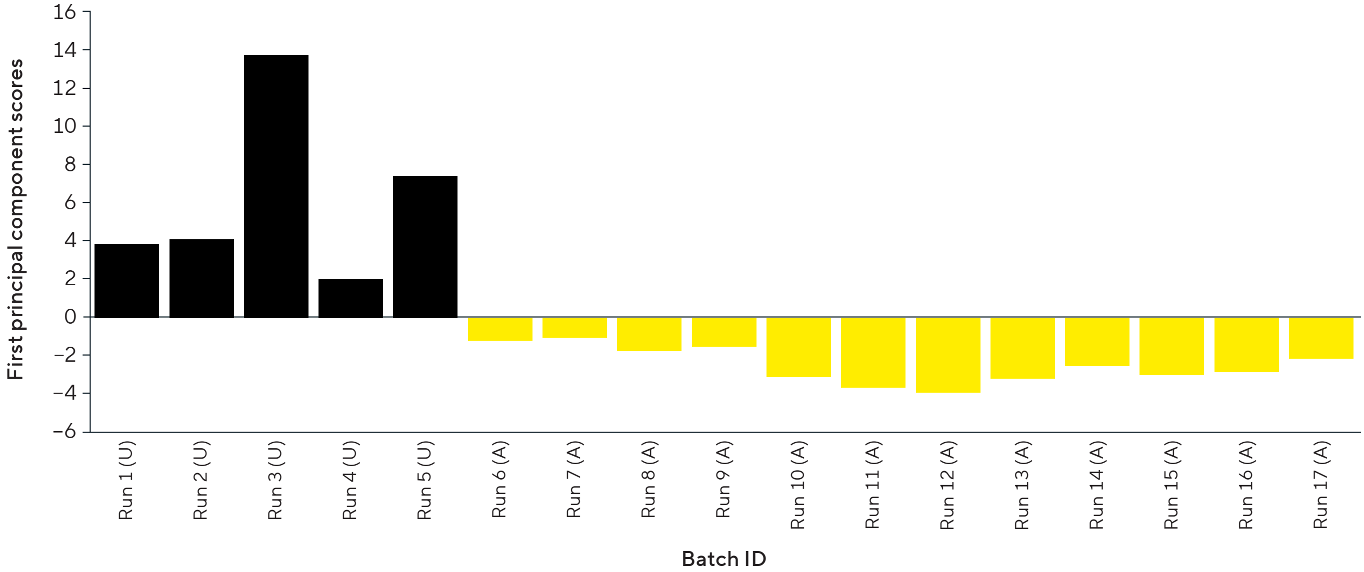


Figure 5: Sorted score contribution plot for two groups of acceptable and undesirable transitions

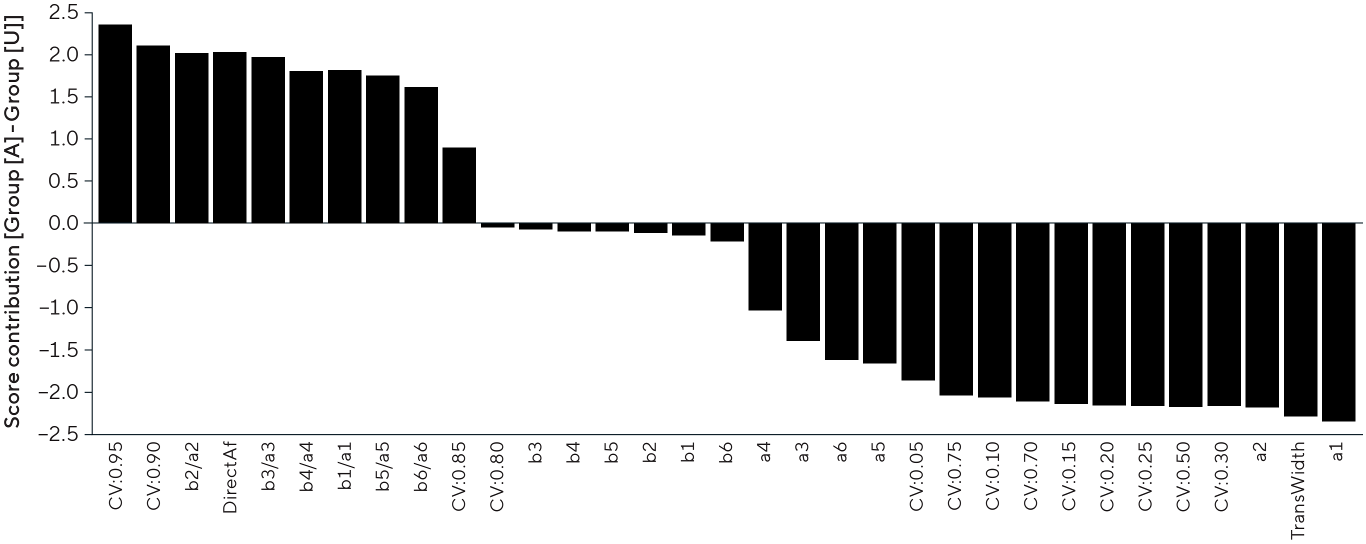


Figure 6: DTA a1 **(A)**, DTA threshold 0.95 **(B)**, DTA TransWidth **(C)**, and DTA DirectAf **(D)** colored by the selected group

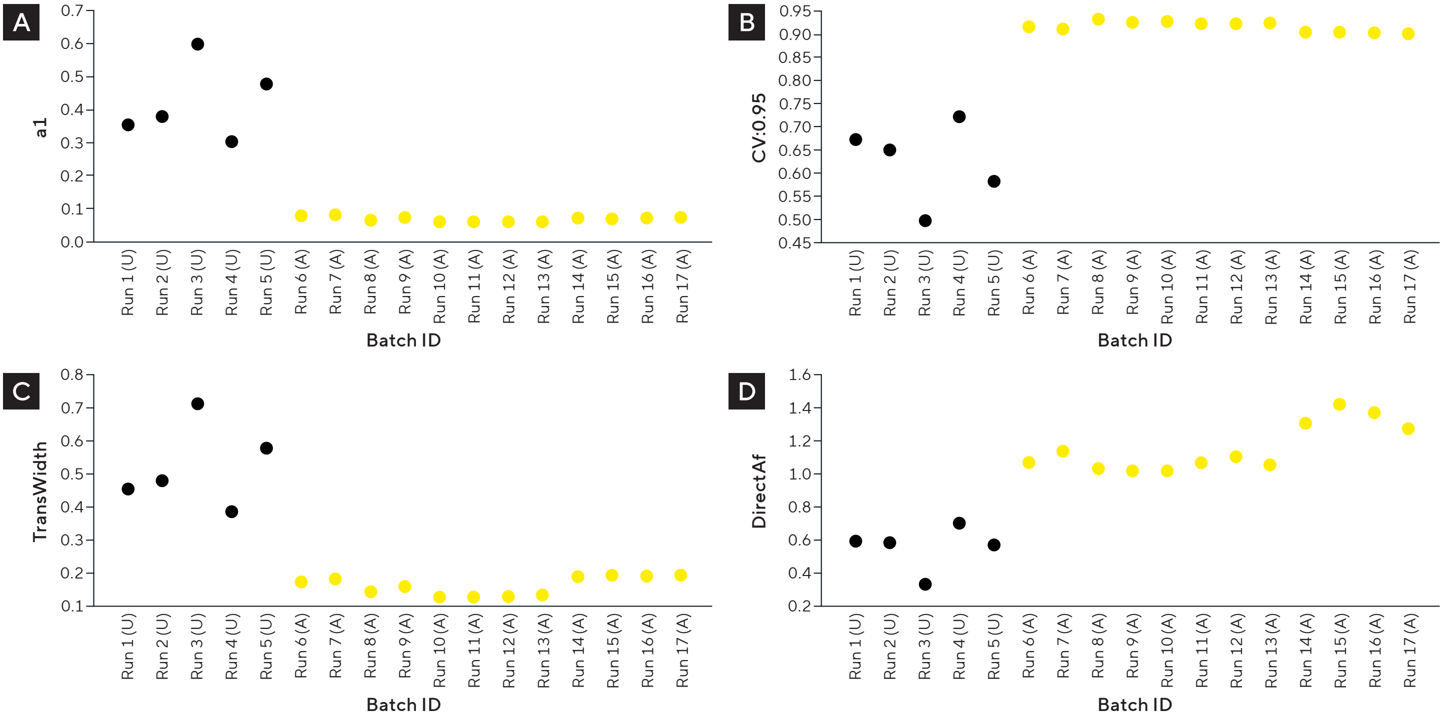
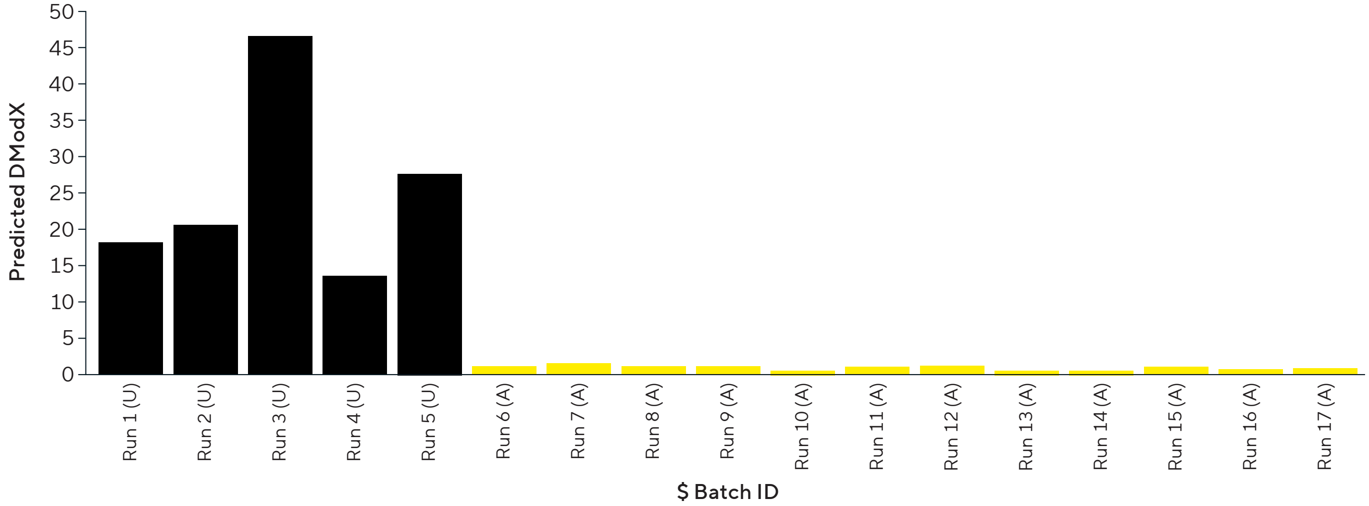


Figure 7: DModX for 1 transitions in the PCA model built using acceptable transition profiles



In Figure 6, DTA a1 and DTA threshold 0.95 are depicted alongside DTA TransWidth and DTA DirectAf to demonstrate that the SIMCA® score contribution plot is a suitable tool for identifying DTA components capturing differences in transition profiles.

After demonstrating the MVDA-DTA approach for segregating the two groups of transitions, a second PCA model was built using only the acceptable transitions. The aim was to assess the model's ability to identify undesirable transitions as outliers using SIMCA® MVDA-DTA outlier detection tools (DModX).

Exposure of the 17 transitions to the second model confirms that the MVDA-DTA outlier detection tool offered by both SIMCA® and SIMCA®-online would identify all five undesirable transitions with significantly high DModX values relative to the low DModX values of the acceptable transitions. Figure 7 shows the DModX plot for the 17 transitions.

In summary, the first case study demonstrates that the MVDA-DTA approach can differentiate between normal and abnormal transitions, which translates to normal and abnormal process behavior.

Case Study 2: Using DTA to classify batches by product quality

Biopharmaceutical manufacturing process data for 55 chromatography batch runs were provided to assess the MVDA-DTA approach using SIMCA®. The process SME had already identified 12 batches as undesirable based on product quality metrics, confirming the remaining 43 batches for product release. Post-column conductivity profiles of the storage phase were used to investigate the ability of MVDA-DTA to segregate undesirable batches from acceptable ones.

Figure 8 shows the conductivity (mS/cm) versus CV (L) profiles for the storage phase.

First, a PCA model using DTA components of the 55 profiles was built, and score contributions for the first principal component were depicted using SIMCA®. Figure 9 shows that DTA TransWidth could best identify the difference between the two groups with the highest absolute score contribution value.

Figure 8: Profiles of 12 undesirable (U) and 43 acceptable (A) transitions

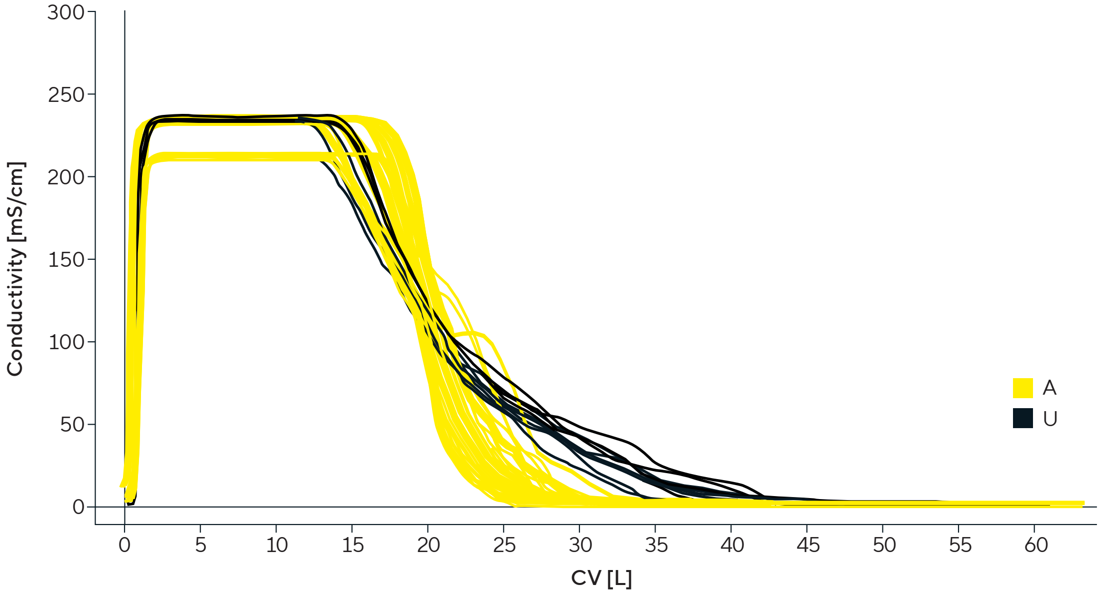


Figure 9: Score contribution plot selecting two groups of acceptable (yellow) and undesirable (black) batches

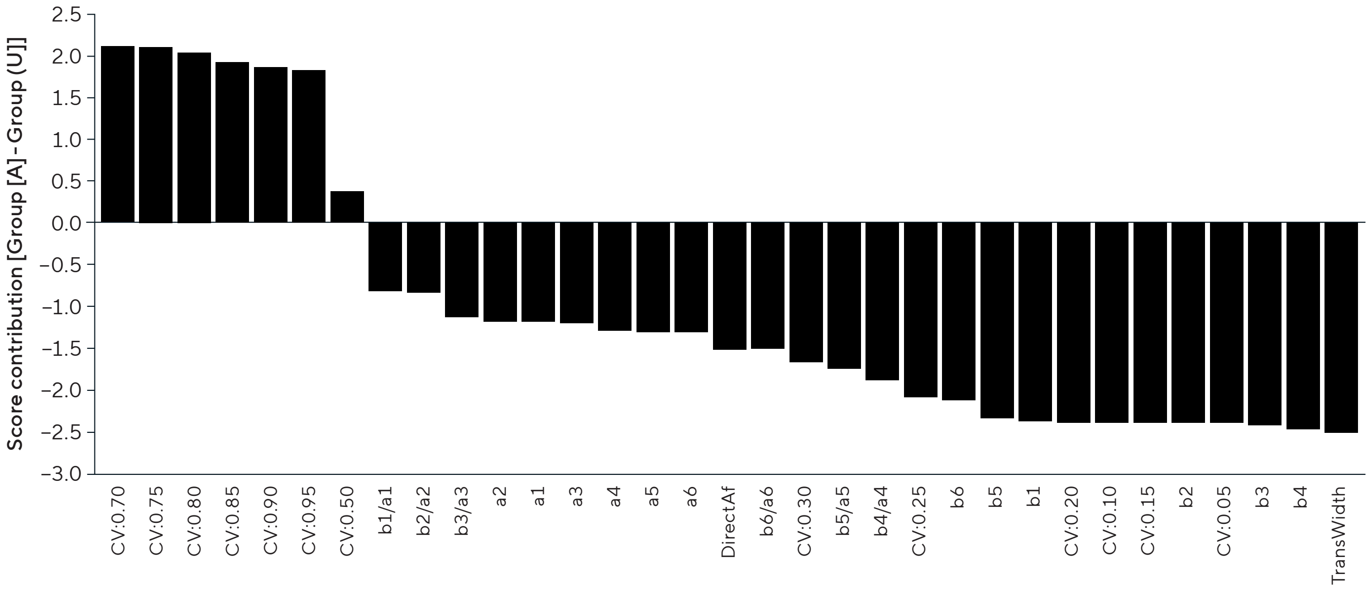


Figure 10 depicts DTA TransWidth values calculated by the DTA SIMCA® Extension in SIMCA®. Undesirable batches are associated with higher DTA TransWidth values compared to those of acceptable batches. This observation confirms the ability of MVDA to summarize informative variations in model structure, as well as DTA's suitability for identifying undesirable batches.

To develop and assess an MVDA-DTA model for process monitoring, a second PCA model was developed in SIMCA® using transition data from the acceptable quality batches. The 55 transitions were exposed to the second model, and DModX values were plotted (Figure 11).

The PCA model with four principal components was able to detect undesirable batches with higher DModX values compared to acceptable batches with lower DModX values.

This approach confirms that if the second MVDA-DTA model was applied in an online monitoring scheme by SIMCA®-online, undesirable batches could be detected.

In summary, the second case study demonstrates that the MVDA-DTA approach can effectively classify batches based on product quality.

Figure 10: DTA TransWidth for acceptable (yellow, A) and undesirable (black, U) batches

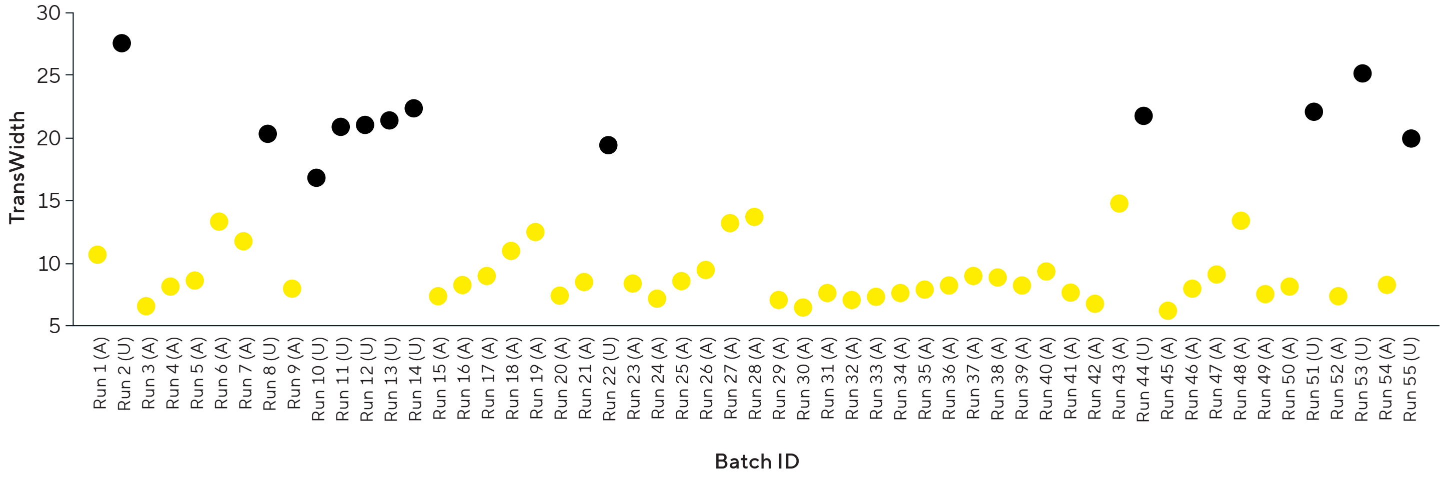
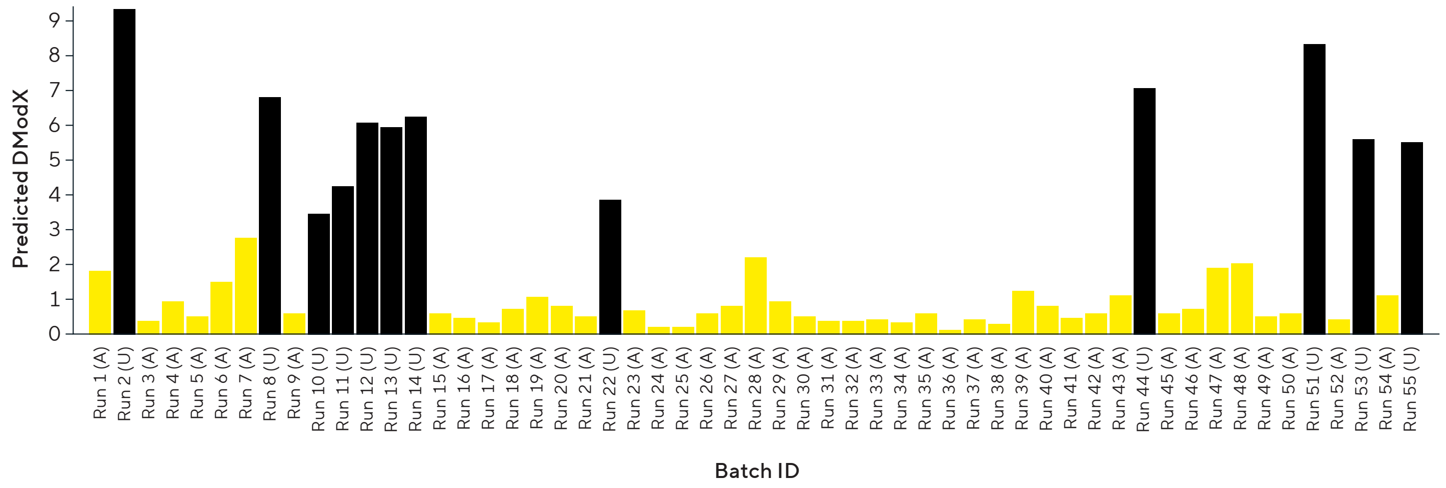


Figure 11: DModX for 12 undesirable and 43 acceptable batches exposed on the DTA-PCA model with four components



Case Study 3: Monitoring resin usage and packing method

Manufacturing chromatography data were provided for six production campaigns, with the column resin replaced at the end of each campaign. There were 20, 28, 20, 20, 16, and 20 batches in the six campaigns, respectively. The process was validated for resin usage in 20 batches. Under an experimental protocol in the second campaign, resin usage was extended to 28 batches. Assessment of the process critical quality parameters did not support the extension of resin use over 20 batches, as quality significantly dropped from the twenty-first run.

The application of MVDA-DTA was investigated using the transition data available for the six campaigns, including the second campaign with experimental runs. In Figure 12, the conductivity transition profiles for all six campaigns are depicted during the equilibration phase. The transitions associated with batches that exceed 20 runs per resin stand out compared to those associated with resin usage of fewer than 20 batches.

As demonstrated in Figure 13, MVDA-DTA in SIMCA® distinguishes batches with more than 20 resin runs from those with fewer than 20. The score values of the first principal component (t[1]) from the PCA model built on DTA variables from equilibration-phase transitions capture this difference.

Figure 12: Conductivity transition profiles for over 120 batches (6 campaigns of around 20 runs each)

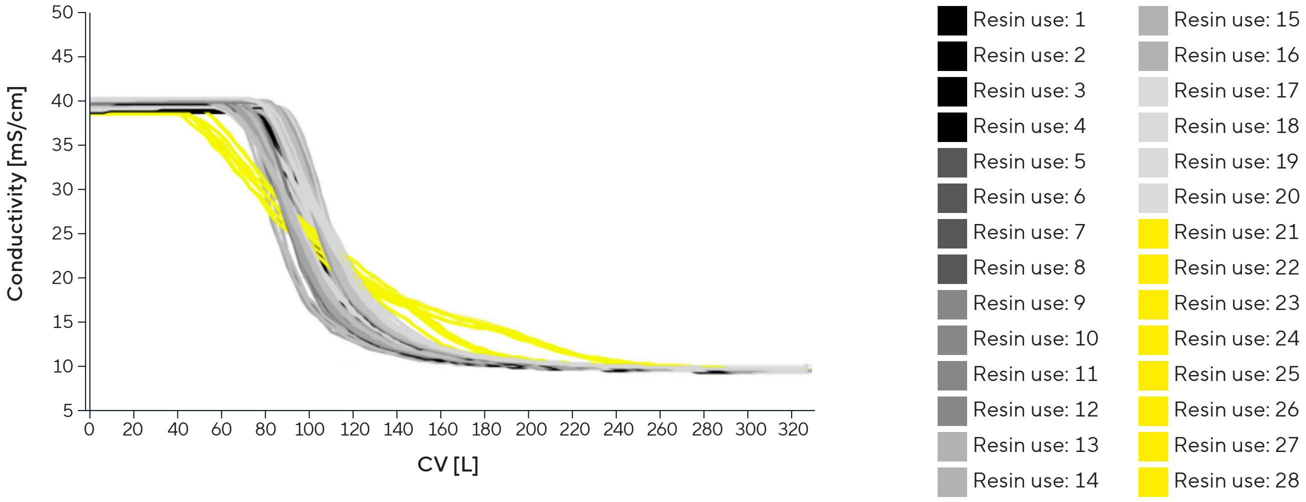
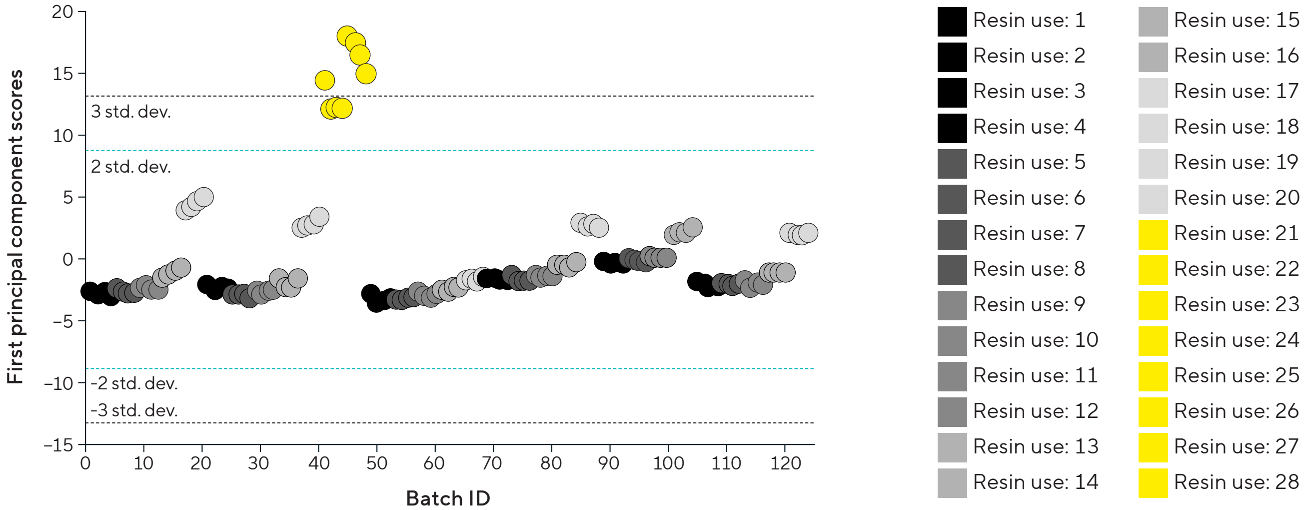


Figure 13: Scores plot for the first principal component of the PCA built on DTA variables



This study demonstrates that variation in column performance can be monitored by observing conductivity transitions. Furthermore, it confirms the practical application of MVDA-DTA as a process monitoring tool for detecting abnormal operational conditions. It is also interesting to observe the increase in first principal component scores for batches with resin usage between 16 and 20 runs. This suggests that MVDA-DTA can be used as a monitoring tool for identifying the optimal resin change point for each ongoing campaign.

Another interesting observation was the clear reflection of resin packing strategies in the DTA CenterPoint (threshold of 0.50). Figure 14 shows DTA CenterPoint values for the more than 120 transitions depicted in Figure 12. Across the sequential batch numbers, six clusters corresponding to the six production campaigns can be identified. The first, third, and sixth campaigns (batches 1 – 20, 49 – 67, and 104 – 124, respectively) have DTA CenterPoints above 100, whereas the fourth and fifth campaigns (batches 68 – 88 and 89 – 103, respectively) have CenterPoints below 100. The process SME confirmed that the first, third, and sixth campaigns used the same resin packing strategy, which differed from the strategy applied in the fourth and fifth campaigns.

For the second campaign, which followed an experimental protocol, a combination of different resin packing strategies was applied.

In summary, this case study demonstrates that the MVDA-DTA approach can be applied to monitor chromatography column resin usage and the packing method.

Case Study 4: Detecting process changes and enhancing process robustness

In manufacturing chromatography, processes are often designed to run a product stream in multiple cycles. Multi-cycle chromatography operations enable higher product quality while reducing resin consumption through smaller-scale operations. In this case study, manufacturing chromatography data for 38 double-cycle (two iterations per batch) runs conducted between 2019 and 2022 were made available. The transition profiles of post-column conductivity (mS/cm) over CV (L) for the resin wash phase are depicted in Figure 15.

Figure 14: DTA CenterPoint values reflecting different column packing strategies

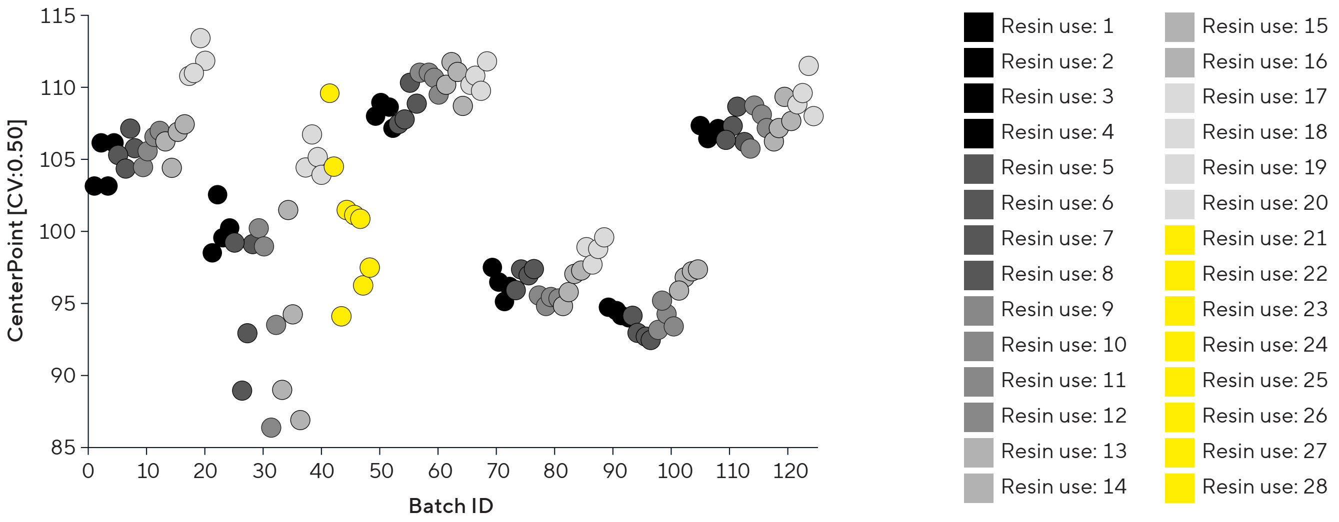


Figure 15: Conductivity transition profiles for 38 double-cycle chromatography runs (76 transitions)

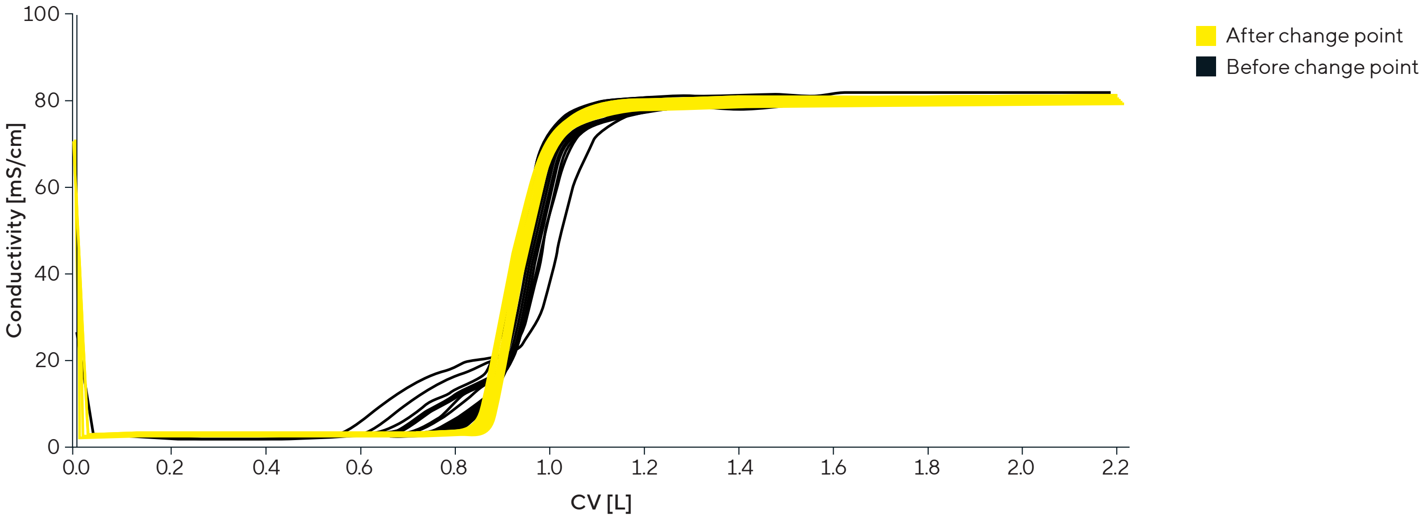
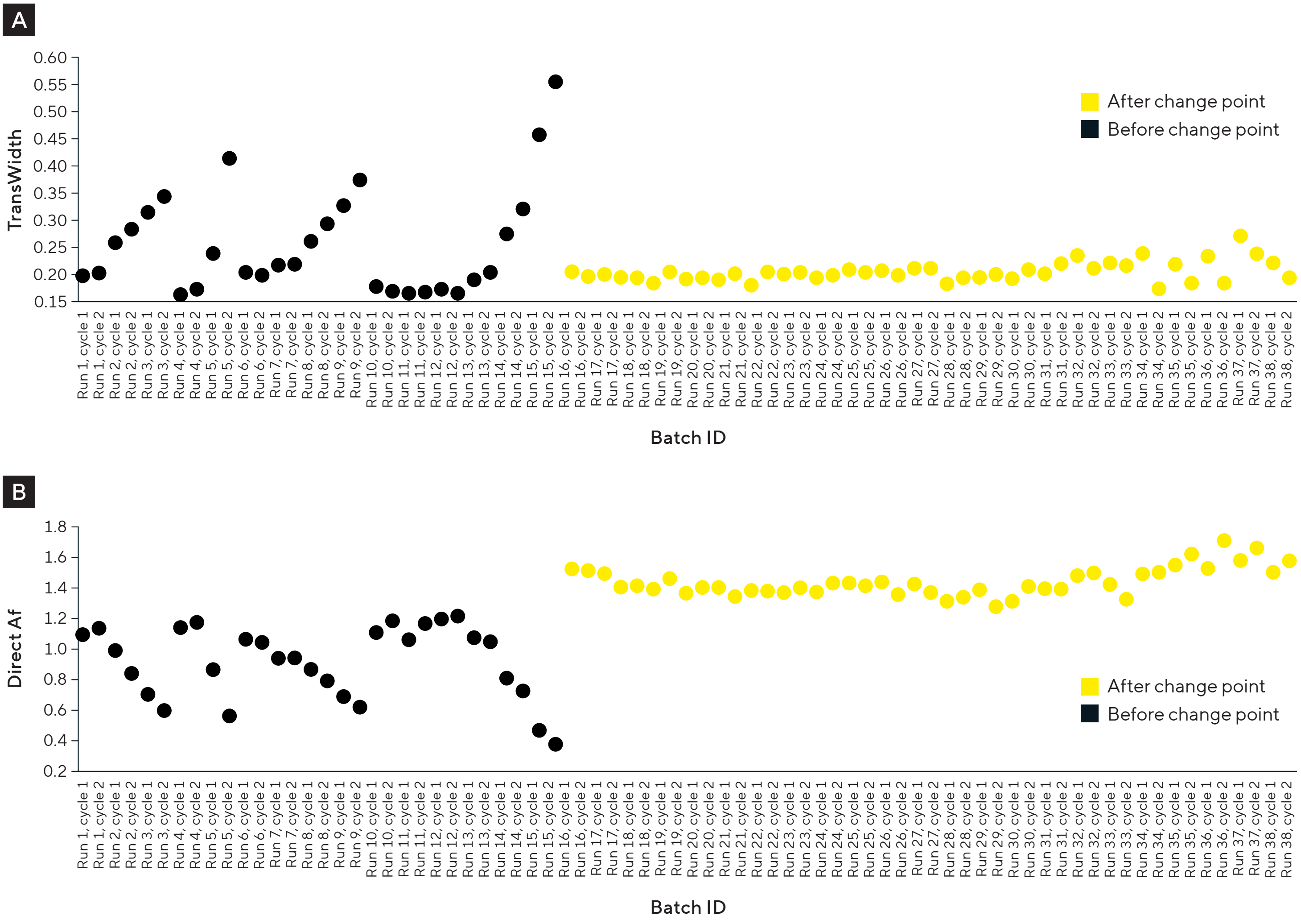


Figure 16: DTA TransWidth **(A)** and DirectAf **(B)** for the 38 batch runs (76 profiles) between 2019 and 2022



In Figure 16, DTA TransWidth and DTA DirectAf are depicted for the batch runs spanning approximately two years of production. In both plots, a change point at the sixteenth batch run is observable. This change point aligns with the first batch run after a process change was implemented to target reduced column bed instability in earlier batches. The column compression factor was increased to enhance process robustness and extend the operational lifetime of a column pack.

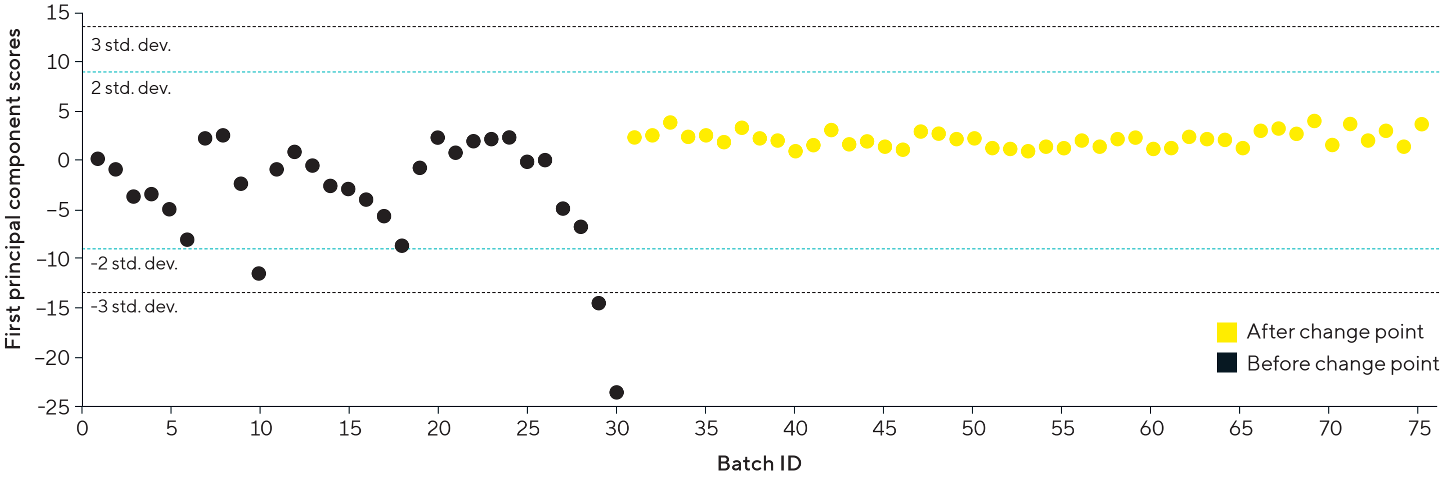
Figure 16 illustrates that DTA aligns with SME process knowledge. Before the sixteenth batch run, batch-to-batch variability was higher than after the process change point, confirming that increasing the column compression factor enhanced process robustness. DTA was used for post-study analysis of the data; however, if it had been applied in real-time for batch-to-batch column performance assessment, earlier detection of the variability could have prompted earlier intervention, reducing resin cost and increasing consistency. Once again, a multivariate PCA model summarizing DTA variables offers a powerful tool for assessing batch-to-batch column performance in SIMCA® and SIMCA®-online.

Figure 17 illustrates the scores of the batch runs, summarizing DTA variables using a single-component PCA model.

The process change point of batch run 16 is evident in Figure 17, confirming the effectiveness of the process monitoring scheme using MVDA-DTA by SIMCA® and SIMCA®-online.

In summary, this case study demonstrates that the MVDA-DTA approach can be applied to detect process changes and enhance process robustness.

Figure 17: Scores plot for the first principal component (t[1]) PCA model using DTA variables



Summary

The benefits of using transition analysis over the traditional salt-plug test for batch-to-batch chromatography column performance assessment were reviewed. DTA is a straightforward procedure that requires little data processing, making it an ideal new standard for monitoring the condition of chromatography columns.

It was demonstrated that DTA metrics, when summarized by an MVDA model, are effective in detecting abnormal or unwanted operational conditions. The promising application of the MVDA-DTA approach was highlighted with data from four different biopharmaceutical companies. Each case study, focusing on a different aspect of the process monitoring scheme, demonstrates the success of the method as an effective tool for various real-world scenarios.

References

1. Fetterolf, D. M. (2009). Column chromatography. *Journal of Validation Technology*, 15(2), 43. https://www.proquest.com/openview/dd75dbacd7be04a3887fd45f8d6e2f4b/1
2. Teeters, M. A., & Quiñones-García, I. (2005). Evaluating and monitoring the packing behavior of process-scale chromatography columns. *Journal of Chromatography A*, 1069(1), 53–64. https://doi.org/10.1016/j.chroma.2005.02.051
3. Hofmann, M. (1998). A novel technology for packing and unpacking pilot and production scale columns. *Journal of Chromatography A*, 796(1), 75–80. https://doi.org/10.1016/S0021-9673(97)00727-9
4. Gondkar, S., Manudhane, K., Amritkar, N., Pai, A., & Lali, A. (2008). Effect of adsorbent porosity on performance of expanded bed chromatography of proteins. *Biotechnology Progress*, 17(3), 522–629. https://doi.org/10.1021/bp010029m
5. Moscariello, J., Purdom, G., Coffman, J., Root, T. W., & Lightfoot, E. N. (2001). Characterizing the performance of industrial-scale columns. *Journal of Chromatography A*, 908(1–2), 131–141. https://doi.org/10.1016/s0021-9673(00)01062-1
6. Cui, Y., Huang, Z., & Prior, J. (2018). Using direct transition analysis in chromatography. *BioPharm International*, 31(1), 34–40. https://www.biopharminternational.com/view/using-direct-transition-analysis-chromatography
7. Larson, T. M., Davis, J., Lam, H., & Cacia, J. (2003). Use of process data to assess chromatographic performance in production-scale protein purification columns. *Biotechnology Progress*, 19(2), 485–492. https://doi.org/10.1021/bp025639g
8. Harrison, R. G., Todd, P., Rudge, S. R., & Petrides, D. P. (2015). Bioseparations science and engineering (2nd ed.). New York: Oxford University Press. https://global.oup.com/academic/product/bioseparations-science-and-engineering9780195391817?cc=gb&lang=en&
9. Levenspiel, O. (1998). *Chemical reaction engineering* (3rd ed.). John Wiley & Sons.

10. Savitzky, A., & Golay, M. J. E. (1964). Smoothing and differentiation of data by simplified least squares procedures. *Analytical Chemistry*, 36(8), 1627–1639. https://doi.org/10.1021/ac60214a047
11. Macaulay, F. R. (1931). Introduction to "The smoothing of time series". New York: National Bureau of Economic Research.
12. Powell, J. L., & Newey, W. K. (1987). Asymmetric least squares estimation and testing. *Econometrica*, 55(4), 819-847. https://www.jstor.org/stable/1911031
13. Wold, S., Esbensen, K., & Geladi, P. (1987). Principal component analysis. *Chemometrics and Intelligent Laboratory System*s, 2(1-3), 37–52. https://doi.org/10.1016/0169-7439(87)80084-9
14. Kim, K., Lee, J.-M., & Lee, I.-B. (2005). A novel multivariate regression approach based on kernel partial least squares with orthogonal signal correction. *Chemometrics and Intelligent Laboratory Systems*, 79(1–2). https://doi.org/10.1016/j.chemolab.2005.03.003
15. Stenlund, H., Johansson, E., Gottfries, J., & Trygg, J. (2009). Unlocking interpretation in near infrared multivariate calibrations by orthogonal partial least squares. *Analytical Chemistry*, 81(1), 203–209. https://doi.org/10.1021/ac801803e
16. Trygg, J., & Wold, S. (2002). Orthogonal projections to latent structures (O-PLS). *Journal of Chemometrics,* 16(3), 119–128. https://doi.org/10.1002/cem.695
17. Bylesjö, M., Rantalainen, M., Cloarec, O., Nicholson, J. K., Holmes, E., & Trygg, J. (2006). OPLS discriminant analysis: Combining the strengths of PLS-DA and SIMCA classification. *Journal of Chemometrics,* 20(8–10), 341–351. https://doi.org/10.1002/cem.1006
18. Sartorius. (2023). SIMCA®—Multivariate data analysis software. https://www.sartorius.com/en/products/process-analytical-technology/data-analytics-software/mvda-software/simca

Germany
Sartorius Stedim Biotech GmbH
August-Spindler-Strasse 11
37079 Göttingen
Phone +49 551 308 0

USA
Sartorius Stedim North America Inc.
565 Johnson Avenue
Bohemia, NY 11716
Toll-Free +1 800 368 7178

For more information, visit
sartorius.com

Last modified: 5 | 2026