



WHITE PAPER NOVEMBER 2022

**Efficient and reliable**  
**UHPLC pump maintenance**  
Self-diagnostics using  
Digital Twin

**Better Sample Care.**

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# Table of contents

- 1. Overview**
- 2. UHPLC pump symptoms**
- 3. Current approach**
- 4. Diagnostics 2.0**
  - Digital Twin & autonomous diagnostics
  - Recommendations & fixing instructions
  - User benefits
- 5. Future-proof**

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# 1. Overview

Ultra High Performance Liquid Chromatography (UHPLC) pumps are used in laboratories all over the world. These instruments can pump mobile phase solvents with a very accurate flow rate over a large pressure range.

To meet nowadays laboratory requirements and assure this excellent precision performance the flow rate of the pump has to be constant over the pressure range (0 - 1300 bar). The smallest deviation in pressure and/or flow can be an indication of an (upcoming) defect in which the reliability of the analysis of the samples is at stake.

To ensure good, stable pump performance and maximize instrument uptime, it is necessary to closely monitor the pump's operation. That is why Spark Holland is implementing a state-of-the-art diagnostic tool for its UHPLC pumps that makes it possible to carry out accurate diagnoses and detect if a component of a system is (not) operating properly. The diagnostic tool is created using Digital Twin technology, developed in collaboration with industry experts, and allows for monitoring of the most important Key Performance Indicators.

The patent pending diagnostic tool will bring substantial analytical and problem-solving advantages and represents next level customization. This autonomous intelligence will enable service engineers to find, locate and fix problems quicker, more easily and accurately, and improve instrument uptime significantly.

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## 2. UHPLC pump symptoms

An UHPLC system consists of many components and performance issues can arise, often caused by known wear parts, like check valves and sealings, or aging of the system during lifetime. Most of the common symptoms of UHPLC pumps concern:

- shifting retention times
- baseline drift
- pressure fluctuation
- lower column back pressure

The challenge for a service engineer is to efficiently identify the most likely cause of each symptom, but how?

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## 3. Current approach

Many service engineers opt for corrective and/or preventive maintenance, with or without certain diagnostics, for UHPLC pumps.

Corrective or reactive maintenance is failure-oriented and aimed at quick recovery when a UHPLC pump is not working properly and the operation of a UHPLC system is compromised. Troubleshooting guides can help to identify, isolate and correct an issue. However this process can be time consuming and disappointing, when it involves trial and error. Lack of technical knowledge, may even result in the unnecessary replacement of parts that are not defective. Thus, for instance, an entire pump head may be replaced when only the seal, as a wearing part, would need to be replaced. As a result, maintenance becomes more expensive.

Preventive maintenance is planned and scheduled. It can be performed by inspecting a pump more regularly to prevent downtime. It involves inspections according to a maintenance program, at fixed intervals to replace parts before they can cause problems because of wear. The interval depends on system usage but is usually set to once per year out of convenience which might not be sufficient for all users. In addition, this periodic check requires more frequent testing in a specific test setup with operational interruption and, like corrective maintenance, accurate record keeping.

Preventive maintenance kits concern:

- high pressure seals
- low pressure seals
- check valves
- solvent filters
- inlet filter
- pistons
- purge valve rotor seal.

Corrective and preventive maintenance can cause unnecessary downtime due to, for example, lagging technical expertise or insufficient maintenance capacity. Also, both types of maintenance require confirmation that the pump performance is according expectation after maintenance. That validation can be obtained with Diagnostics 2.0.

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## 4. Diagnostics 2.0

UHPLC systems are complex and it is a great challenge for a service engineer to master all parts of the system, both in terms of operation and troubleshooting. The UHPLC pump alone requires a great deal of technical knowledge, which is not always present. This also applies to the troubleshooting tools that are commonly used. The level of knowledge and skills of the service engineer is leading for successful diagnostics and troubleshooting.

Service engineers and maintenance departments are always looking for better ways to guarantee or restore the performance of UHPLC systems. This means easier, quicker and more reliable ways to keep the systems and its modules operational and minimize unnecessary downtime. In short, they want the best reliability strategy for maximizing uptime of their UHPLC pumps.

Based on her years of experience with Digital Twin, Spark Holland concludes that her diagnostic tool for autonomous testing is a valuable and very reliable addition to existing methods of maintenance and diagnostics.

A Digital Twin is a highly accurate, virtual working model of an intended system (product or service) in a given environment. Within the innovative manufacturing industry, a Digital Twin is widely used today. A Digital Twin is constructed based on the same natural laws and principles as a system in the real world. The way a Digital Twin behaves in its virtual world is almost identical to its physical counterpart.

Designing with a Digital Twin has great advantages. The system design can be optimized by engineers at an early stage, with or without customer feedback, before it is put into production. Furthermore, it enables several design concepts to be virtually validated in advance. This saves time and money, also because fewer physical prototypes are needed. In short, the engineering process is more efficient while at the same time it is more thorough. This also applies to further development and modification of the product/system. Another advantage is that the development of hardware and firmware can run in parallel with the mechanical design, which again saves time.

A Digital Twin of a product consists of data (the digital base) and models related to requirements, form, structure, calculations, specifications and simulations of a product. At Spark

Holland, the mechanical domain of a Digital Twin is developed at the start of the mechanical design to validate its ability to meet product requirements. With the system description that the Digital Twin offers at that stage, engineers are able to simultaneously start with the design of electronics and firmware. When the design has reached the required level of detail, prototypes can be produced and tested. By collecting data from physical prototypes, for example on flow and pressure, the last details of the Digital Twin are tuned in order to represent the physical system as accurately as possible. With this approach the Digital Twin forms an additional design layer, which helps engineers analyze a system more thoroughly and foresee problems before they occur.

In addition to the benefits of developing a Digital Twin during the design process, the Digital Twin also allows to perform a multitude of experiments in a short time. Furthermore, a Digital Twin is capable to consistently and repeatedly simulate the system behavior with worn wear parts in a controlled environment, which is difficult to achieve on a physical system. These properties allow engineers to develop state-of-the-art diagnostic tools based on machine learning. These tools help field service engineers to faster locate worn components causing an underperforming system, saving time and costs.

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## Digital Twin & autonomous diagnostics

In its continuous ambition for optimizing UHPLC modules, Spark Holland uses a Digital Twin model. This model facilitates the development of UHPLC pumps in two ways:

- Design: to optimize the system design in terms of firmware, mechanics, etc.,
- Diagnostics: optimizing the diagnostic performance.



Spark Holland has developed its diagnostic tool to make pump system information more accessible to service engineers. Because the diagnostic tool was developed with Digital Twin technology, Spark Holland can introduce an efficient and reliable way of diagnostics. The separate tool enables automatic monitoring of pump operation within a control system.

Using this autonomous diagnostics tool, a service engineer or user can diagnose whether a pump is operating within the parameters of that equipment, or the manufacturer's prescribed performance objectives. The diagnostic tool validates whether the observed values of the physical system match the calculated results of the model.

During the diagnostic process, analysis takes place with the help of machine learning. This package contains data for almost 100 different Key Performance Indicators (KPIs) and recognizes abnormalities or patterns of error. Spark Holland has made the data very accessible. The output is presented from a PC in an understandable form to the user. The service engineer doesn't need to analyze a log file, but can suffice with on-site review of the analysis made by the diagnostic tool of the detailed data.

## Recommendations and fixing instructions

The diagnostics tool not only helps analyze information very quickly, but also locates any inaccuracies or discrepancies, for example the anomalous behavior of a check valve, and advises the user how to fix it (recommendations and instructions).

## Maintenance procedure using Diagnostics 2.0

Using the diagnostic tool the UHPLC pump maintenance procedure becomes as follows:

1. Diagnostic routine: select test and click 'start' to open the wizard that interactively guides you through two steps:
  - a. Initialization: pump initialization and check parameters (sensors, drives, cables etc.) in order to determine if the diagnosis can be performed.
  - b. Analysis: automatic priming and purging, increase flow rate, pump during several minutes, determine secondary seal leakage, extract logfile and run diagnostics & detect patterns.
2. Results: check the automatically presented feedback with visual indication of the location of the failing part.
3. Recommendations: click 'next' to get instructions for solving the problem.
4. Follow-up: implement the recommendations by, for example, calibrating the pump and replacing parts.
5. Validate: validate the solution by running steps 1 to 4 again until the problem is solved.

The tests are performed with water and total test times takes 15-20 minutes.

## User benefits

Spark Holland's diagnostic tool takes troubleshooting off the hands of engineers as it takes over the interpretation of the pump's actual operation. Troubleshooting takes many recurring, standard steps out of the hands of the service engineer, allowing him to focus more (efficiency) on fixing rather than analyzing an anomaly or problem.

The main user benefits of the Spark Holland diagnostic tool are:

- Locating problems and solutions,
- Better understandable and comprehensible data (easy readable interface),
- Faster and easier troubleshooting and fixing,
- Reduce unnecessary part exchange,
- Higher uptime.



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## 5. Future-proof

By applying Digital Twin technology for its UHPLC pumping systems, Spark Holland supports service engineers in their efforts to make the maintenance processes more effective and reliable (> 90% accuracy thanks to the smart use of lots of available data) and increase system uptime.

The diagnostic tool can be used as an additional tool for maintenance and troubleshooting a problem, but also provides capabilities for future real time diagnoses and forecasts (predictive maintenance), as well as for integration into software programs of OEM partners. In other words, the diagnostic tool is future-proof for anyone who wants the best reliability strategy for UHPLC pumps. •

### Patent pending

Spark Holland has a patent pending for the diagnosis of a controlled LC pump unit:

- Patent pending diagnostics EP 3 992 626 A1
- US20220128522A1 US20220128522A1 Training a neural network processor for diagnosis of a controlled liquid chromatography pump unit - Patent View - PatSnap

Training a neural network processor is described for providing diagnostic information of a controlled liquid chromatography pump unit. The training includes executing a sequence of operations wherein the neural network processor is trained with input signals obtained from a simulated version of the controlled liquid chromatography pump unit and associated sensors, while modifying the simulated version of the liquid chromatography pump unit to a pump fault simulation signal. Dependent on a value of the pump fault simulation signal, the simulated version of the liquid chromatography pump unit simulates operation of the liquid chromatography pump unit free from faults or the operation thereof with one or more pump faults. The trained neural network processor obtained therewith is thereafter integrated with a controlled liquid chromatography pump unit to provide for auto-diagnostic capabilities or used in a separate diagnostic unit for diagnosing one or more controlled liquid chromatography pump units not having auto-diagnostic capabilities.