

Technical Report

IC Solution: Innovative Software that Streamlines Routine Analysis

Katsuaki Koterasawa¹

Abstract:

Ion chromatographs are analytical instruments widely used in test methods specified by various regulations in environmental and related fields. Analytical instruments must not only meet the performance standards required by these test methods, but also enable anyone to perform analyses easily, without confusion, and reliably. IC Solution is routine analysis software designed so that a laboratory manager can preconfigure analysis methods in advance, and users can then perform analyses according to the templates set by the manager, reliably carrying out daily routine analysis tasks, including regulatory compliance testing, regardless of their level of experience. This article describes the key features of IC Solution.

Keywords: Ion Chromatograph

1. Introduction

Amid growing environmental concerns, compliance with various regulations is increasingly required. Ion chromatographs are widely used in test methods specified by various regulations in the environmental field, where they are expected to deliver accurate and highly reliable analytical results. To improve the efficiency and reliability of analysis, it is essential to create an environment in which users can operate the instrument easily.

IC Solution, a routine analysis software program, was developed to meet these needs. This software is designed to allow users to easily perform analyses based on analysis methods preconfigured by a laboratory manager. This approach allows anyone to run consistent analyses on a routine basis, including for regulatory compliance testing. This article describes the main features of IC Solution and its key benefits in detail.

2. Streamlining Analysis Workflows with IC Solution Routine Analysis Software

IC Solution is an effective tool for simplifying analysis operations. The laboratory manager uses IC Solution to create method templates with preconfigured analysis conditions, acceptance criteria, and other parameters, then users of IC Solution simply select and run the relevant analysis template. The user interface and features included with IC Solution are optimized for ease of use to improve working efficiency and ensure reliable and efficient analysis (Figure 1).

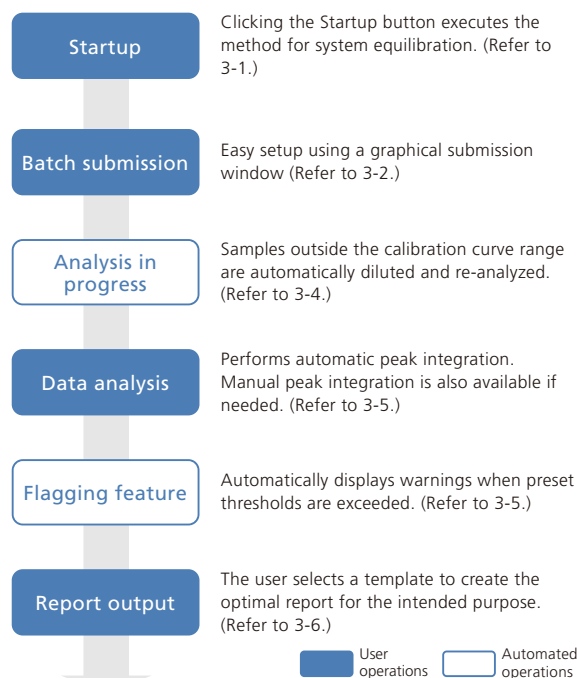


Figure 1: Analysis Workflow with IC Solution

Figure 2 shows the main window of IC Solution. This main window displays: (1) system status, (2) analysis parameters, (3) batch submission status, and (4) analysis results in a simplified chart format. Clicking the (5) Startup button or the (6) Start Analysis button starts each operation. The solvent delivery pump, column oven, and other components can be controlled individually from the (7) Direct Control pane. Clicking the (8) Submit Batch button opens a separate window to add sample batches to an analysis. This window can be used to add additional batches to the end of a batch queue, but can also add batches at any position in the batch queue during an ongoing analysis. Also, clicking the Analysis Application Startup button launches a dedicated analysis application for processing data.

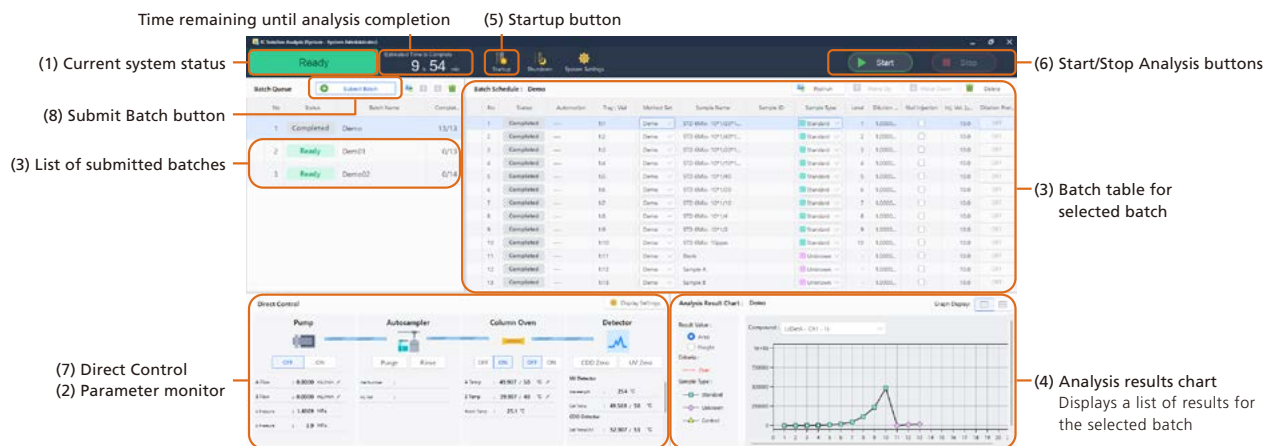


Figure 2: IC Solution Main Window

3. Operational Flow in IC Solution

3-1. Startup (Pre-Analysis System Equilibration)

In IC Solution, by setting a startup method in advance, users can perform pre-analysis procedures such as auto-purge, column warm-up, and column equilibration simply by clicking the Startup button. Nexera™ IC also comes with FlowPilot, an in-built feature that automatically adjusts flowrates depending on the column oven temperature. This feature allows column equilibration to be executed automatically without excessive pump pressures (Figure 3).

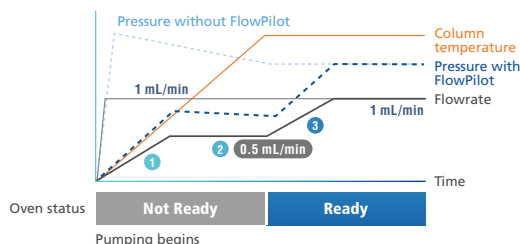


Figure 3: FlowPilot Overview

After pumping begins, the flowrate is gradually increased, and until the column oven temperature stabilizes, pumping is performed at half the set flowrate. Once the oven temperature reaches the target temperature, the flowrate is increased again until it reaches the target flowrate.

3-2. Batch Submission

Batch analysis schedules can be created directly in IC Solution using its intuitive graphical user interface (Figure 4).

In addition, settings for the automatic sample dilution feature available with the Nexera IC autosampler can be easily configured. Clicking on the Dilution Pretreatment button next to each sample displays the configuration window, where automatic dilution/analysis can be configured by simply entering the position of the stock solution vial and a dilution factor. As sample dilution is performed in a separate empty vial, the user must also specify the tray and vial number of an empty vial in the batch schedule.

If an urgent sample is received during analysis, it can also be inserted after the current analysis or batch is complete. By giving the batch the same name as the currently running batch and checking the [Perform Analysis on Priority] checkbox, the sample can be inserted into the next line of the ongoing analysis.

3-3. Starting Analysis

Once a sample batch is submitted for analysis, clicking the Start Analysis button starts the analysis. If the system is still starting up, analysis can also be scheduled to start automatically once startup is complete.

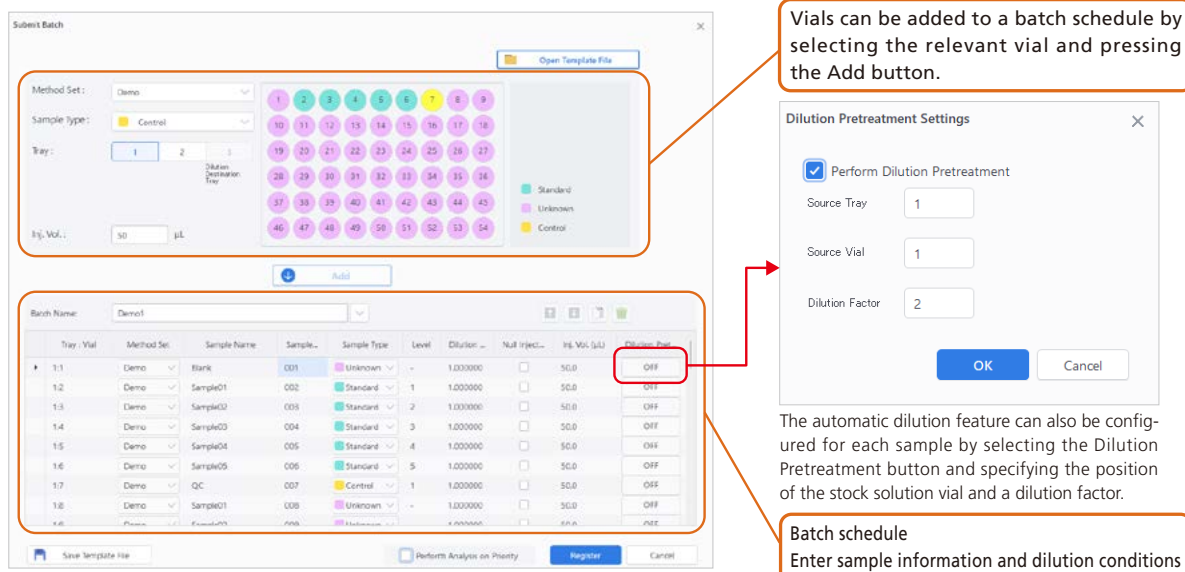


Figure 4: Batch Submission Window

Select a vial number in the top half of the window, click Add to add it to the batch schedule, then enter the sample information and submit it.

3-4. During Analysis

Automatic Identification, Automatic Dilution, and Reanalysis of High-Concentration Samples

IC Solution automatically detects when the ion concentration in a sample exceeds the range of the calibration curve, uses the autosampler's automatic dilution feature to dilute the sample to a concentration within the calibration curve range, then repeats analysis of the diluted sample (Figure 5).

IC Solution can automatically determine the dilution factor from the signal intensity, so no user operation is required. During data analysis, IC Solution recalls the dilution factor and uses it to calculate and display the original concentration.

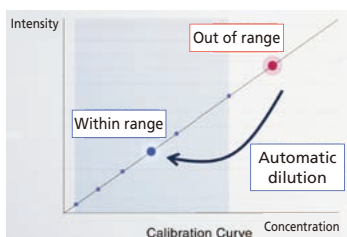


Figure 5: When a sample cannot be quantified because it falls outside the calibration curve range, it is automatically diluted by the autosampler to within the calibration curve range, allowing quantification by re-analysis of the diluted sample.

To prevent carry-over of high-concentration samples outside the calibration curve range, flow lines and the autosampler can be rinsed and a blank sample check can be performed before re-analysis of the diluted sample.

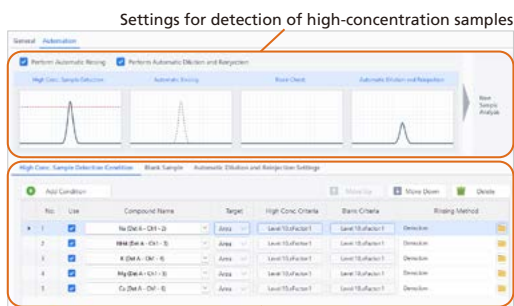


Figure 6: Configuration Window for System Response when a High-Concentration Sample is Detected

Configures ion concentration thresholds and the system response when a threshold is exceeded, such as whether to run a cleaning method or perform dilution/re-analysis.

Analysis Results Chart

Once analysis begins, quantitative results are displayed in real time in a chart in the bottom right of the main window (Figure 7). The charts allow rapid review of the results of continuous analyses of standard, QC, and unknown samples (peak area or height).

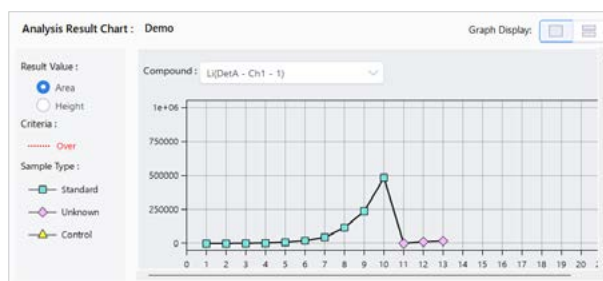


Figure 7: Results Chart

The chart displays quantitative results for each compound from standard, QC, and unknown samples.

3-5. Data Analysis

IC Solution comes with software specifically designed for analyzing quantitative data. The software displays data sets summarized and grouped in one location for easy viewing of quantitative values, chromatograms, and calibration curves (Figure 8).

Flagging Feature

IC Solution also includes a flagging feature that flags abnormal values based on preconfigured thresholds. This feature has a wide range of applications. For example, it can be used to determine whether analysis has been performed correctly based on percentage error at each point on a calibration curve or percentage error in QC analysis.

The flagging feature can also be used with unknown samples to determine whether the concentration of the target ion in each sample falls outside a user-specified reference concentration. Because standards for calibration curve error and QC analysis error are sometimes specified in official methods such as the Water Supply Act, this feature makes it easy to identify abnormal results.

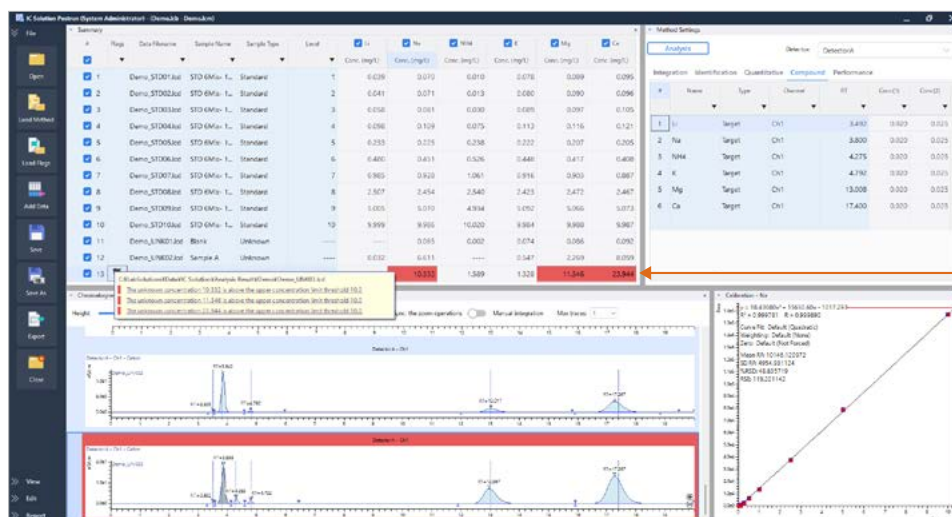
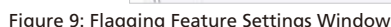


Figure 8: Main Window of the Analysis Application
Can display quantitative values for each sample as well as multiple chromatograms.

Flagging feature: Evaluates each compound in each sample against preconfigured thresholds. Flags are displayed in the flag column of the results table. Placing the mouse over a flag displays a pop-up showing which threshold triggered the flag.

As a result, the system can support various reference criteria, such as percentage error thresholds for calibration curves and QC samples, and an upper concentration limit for unknown samples.



Here, the percentage error threshold for the quantitative value of the standard sample is set to 20 %.

IC Solution includes a summary reporting feature that outputs measurement results. IC Solution offers several templates, including summary reports organized by sample and target ion type; one example is introduced here.

Quantitative results table: This report template compiles the results from all analyzed samples into a single table. This template is suitable when only quantitative values from a series of analyses need to be output. Calibration curves and chromatograms can also be output together (Figure 10).

To improve the efficiency and reliability of analysis using ion chromatographs, it is essential to provide a user-friendly operating environment.

IC Solution is routine analysis software designed to allow its users to conduct analysis simply and reliably based on analysis methods configured in advance by a laboratory manager. This approach allows anyone, regardless of experience level, to reliably perform routine analysis, including regulatory compliance testing.



(Left: Page showing a quantitative results list and part of a calibration curve; Right: Page showing chromatograms from standard sample analysis of six cations (Li^+ , Na^+ , NH_4^+ , K^+ , Mg^{2+} , and Ca^{2+}))

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