

A Physics-Informed Inverse Problem for Tracking Gas Chromatography Column Degradation

Antoine Riaud¹, Balint Toth¹, Yannick Maret¹, Kai Hencken¹

¹ ABB Corporate Research Switzerland, Segelhofstrasse 1K, 5405 Baden-Dättwil, Switzerland, antoine.riaud@ch.abb.com

Summary:

Many sensing systems require inferring a hidden system state from a distorted waveform. In process gas chromatography, column degradation changes the shape of chromatographic peaks, but the underlying physics is nonlinear and difficult to invert. We cast column health estimation as an inverse problem and solve it with a simple physics informed model. The model links peak asymmetry to Langmuir adsorption and converts the inferred loading behavior into a column health metric. On two years of industrial data from six instruments, this metric tracked aging and separated degraded columns early enough to support predictive maintenance.

Keywords: inverse problems, physics informed modeling, condition monitoring, nonlinear transport, gas chromatography

Background, Motivation and Objective

In many sensing systems, the measured signal depends not only on the excitation, but also on the internal state of the system. Recovering that hidden state from the observed signal is a classical inverse problem. In this report, we view gas chromatography as a nonlinear chemical wave propagation problem: a short gas injection travels through a coated separation column and is detected as a chromatographic peak. Usually, the peak area is used to estimate concentration, but we also show that the peak shape contains information about the condition of the column itself.

As the column ages, its molecular coating and active adsorption sites change. This modifies how analytes interact with the stationary phase and leads to broader peaks, stronger or weaker tailing, and in severe cases carryover that interferes with neighboring compounds. Conventional diagnostics such as theoretical plate number capture part of this degradation, but they do not directly explain why the waveform changes or how those changes relate to the chemistry of the column.

The key physical mechanism is nonlinear adsorption. Under low loading, propagation through the column is close to linear and the peak remains nearly symmetric. Under higher loading, Langmuir adsorption makes the transport nonlinear: part of the concentration front moves faster than the rest of the band, producing steep fronts and long tails that resemble

shock-like wave propagation [1,2]. From a signal-processing perspective, this means that the observed peak is the output of a nonlinear transport system whose parameters depend on the health of the column.

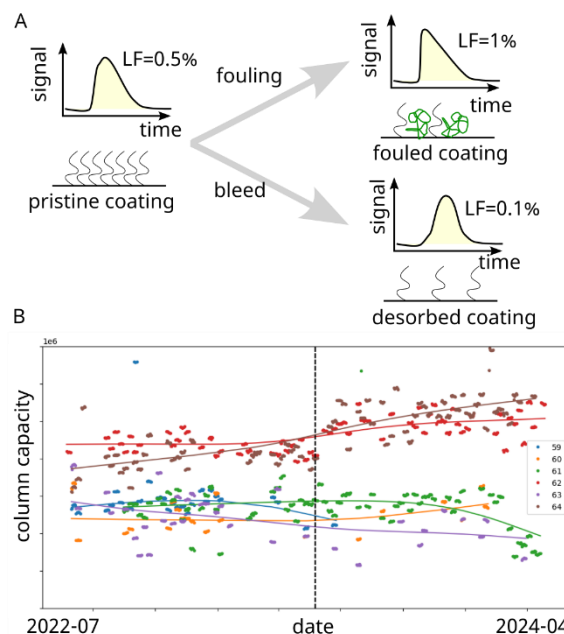


Fig. 1. Physics-informed tracking of gas-chromatography column degradation. Fig. 1.A illustrates a healthy column coating together with two degradation modes, namely stationary phase loss (bleed) and fouling by more active contaminants, and their corresponding peak-shape changes. Fig. 1.B shows the inferred column-capacity trajectories over time, highlighting the early separation of degraded columns from healthy ones. Dashed line indicates maintenance.

The objective of this work is therefore broader than peak fitting used for concentration estimation. We aim to infer column degradation from peak shape by solving a reduced inverse problem: given an observed chromatographic peak, estimate the hidden adsorption state of the column and track how that state evolves over time.

Description of the New Method or System

The exact forward model for this problem is expensive for routine use because it requires simulating nonlinear wave propagation under Langmuir adsorption. That type of model is physically meaningful, but it is not practical to solve repeatedly for every chromatogram in an industrial monitoring workflow. We address this by building a reduced-order surrogate, called HybridMG, that preserves the dominant peak-shape effects of the nonlinear physics while remaining simple to invert.

HybridMG combines two complementary asymmetric peak functions (1): the skewed Gaussian (SG) captures the peak apex well and the exponentially-modified Gaussian (EMG) captures the long tail:

$$\Lambda = \alpha SG + \beta EMG \quad (1)$$

We constrain the family of admissible peak shapes using Langmuir-based simulations of saturated and unsaturated peaks. This step turns peak fitting into an inverse problem with a meaningful solution. Rather than focusing only on the best-fitting curve, the method uses peak asymmetry to infer the loading factor (LF) of the column $LF = n/CC$, with n the amount of sample and CC the column capacity (total amount of available adsorption sites). In order to determine the latter, validation samples of known composition (n) are used, which yields $CC = nLF$. Each chromatogram then yields not just an analyte estimate, but also a direct estimate of the hidden state of the column. In a nutshell, we find a low-dimensional parameterization of the combined shape, which allows to link the different parameters to easily determinable peak parameters.

In practice, the workflow is simple enough for routine monitoring. After baseline correction and peak segmentation, the dominant methane peak is fitted with HybridMG, the loading factor is recovered, and the derived column-capacity metric is tracked over time.

Results

We evaluated the method on more than 1.1 million chromatograms collected over two years from six industrial gas chromatographs monitoring the same gas mixture. For degradation tracking, the first chromatogram of each day was

processed and the dominant methane peak was used to estimate column capacity. The inferred metric separated healthy and degraded columns from the earliest available measurements. Two columns, IP62 and IP64, started with elevated column-capacity values and were later classified as failed within about twelve months, whereas healthy columns remained lower and more stable. This early separation is visible in Fig. 1.B and shows that the hidden degradation state was already encoded in the waveform before conventional maintenance decisions were made.

The significance of the result is broader than gas chromatography. It shows that when a sensor signal is shaped by nonlinear transport, waveform distortion can be treated as information rather than nuisance. A reduced physics-informed model can recover a hidden health variable from the observed signal without repeatedly solving the full nonlinear forward problem. In this work, that hidden variable is linked to column capacity and provides an interpretable health indicator for predictive maintenance.

Overall, the work positions chromatography column monitoring as a signal inversion problem grounded in nonlinear transport physics. The HybridMG model provides a practical bridge between shock-like Langmuir wave propagation and routine industrial diagnostics.

References

- [1] S. Golshan-Shirazi, G. Guiochon, Analytical solution for the ideal model of chromatography in the case of a Langmuir isotherm, *Analytical Chemistry* 60(21), 2364-2374 (1988); doi: 10.1021/ac00172a010
- [2] G. Guiochon, S. Golshan-Shirazi, A. Jaulmes, Computer simulation of the propagation of a large-concentration band in liquid chromatography, *Analytical Chemistry* 60(18), 1856-1866 (1988); doi: 10.1021/ac00169a005
- [3] V.B. Di Marco, G.G. Bombi, Mathematical functions for the representation of chromatographic peaks, *Journal of Chromatography A* 931(1-2), 1-30 (2001); doi: 10.1016/S0021-9673(01)01136-0
- [4] E. Grushka, Characterization of exponentially modified Gaussian peaks in chromatography, *Analytical Chemistry* 44(11), 1733-1738 (1972); doi: 10.1021/ac60319a011