ISSN: 3067-2384
Review Article

World Journal of Sensors Network Research

Intelligent Identification of Multicomponent Mixture Components Using an Artificial Intelligence

Arzu Ibrahimova

Azerbaijan State Oil and Industry University, Baku, Azadliq Aver

***Corresponding author:** Arzu Ibrahimova, Azerbaijan State Oil and Industry University, Baku, Azadliq Aver.

Submitted: 10 September 2025 **Accepted:** 17 September 2025 **Published:** 24 September 2025

https://doi.org/10.63620/MKWJSNR.2025.1045

Citation: *Ibrahimova, A. (2025). Intelligent Identification of Multicomponent Mixture Components Using an Artificial Intelligence. Wor Jour of Sens Net Res, 2(5), 01-03.*

Abstract

This article presents an advanced method for the qualitative and quantitative identification of components in multicomponent mixtures using two densitometers and artificial intelligence (AI). The proposed approach eliminates dependence on chromatographic operating conditions by incorporating a standardized dual-detector system and a mathematical model for determining molecular mass. Regression analysis and neural networks enhance the model's performance, enabling automated, high-precision identification without manual calibration. This article presents an advanced method for the qualitative and quantitative identification of components in multicomponent mixtures using two densitometers and artificial intelligence (AI). The proposed approach eliminates dependence on chromatographic operating conditions by incorporating a standardized dual-detector system and a mathematical model for determining molecular mass. The core equations are enhanced through regression analysis and neural network techniques, enabling automated and high-precision identification without manual calibration. The article introduces Chrom AI ID Pro, a dedicated software platform that integrates signal acquisition, real-time analysis, AI-based predictions, visualizations, and report generation. The system utilizes machine learning algorithms such as Random Forest and MLP Regressor to predict molecular weights based on detector signals and known standard parameters. Comparative simulations demonstrate a significant reduction in prediction error and improved reliability under variable conditions. Experimental data and illustrative examples, including model accuracy comparisons and graphical outputs, are provided to validate the efficiency of the method. The proposed solution is applicable to industrial and laboratory settings where fast, accurate component identification is essential.

Keywords: Chromatographic Identification, Molecular Mass Prediction, Two-Detector System, Standard Identification Column, Densitometric Detectors, AI, Machine Learning (ML).

Introduction

To increase the robustness of component identification under varying chromatographic conditions (e.g., temperature, sorbent type), the study [1] proposed the use of a standard identification column installed after the main column. This secondary column, with fixed and well-characterized parameters, provides uniform passage conditions for all components and enables reliable comparison of signals with reference data, regardless of the primary column configuration. This approach effectively eliminates the influence of external factors, improves accuracy, and facilitates full automation of the analysis process.

Building on this principle, a mathematical model was developed to calculate the molecular mass of each component from the signals obtained by the two densitometric detectors [2-5].. This model underpins the classical two-parametric identification method, which leverages the difference in detector responses before and after the standard column to isolate the effect of molecular mass from other interfering variables.

The classical two-parametric method relies on the following core formula for calculating the molecular mass of component i:

where: $$\mu_i = \frac{A \cdot \mu_{c\_g} - B \cdot \mu_{mix}}{A - B}$$

$$A = \frac{S_{1_i}}{S_{1st} \cdot (\mu_{st} - \mu_{c-g})}, \qquad \mathbf{A} = \frac{S_{2_i}}{S_{2st} \cdot (\mu_{st} - \mu_{mix})}$$

This method has advantages:

- Independence from chromatographic column behavior
- Fast identification process

At the same time has several limitations:

- Sensitivity to noise
- No modeling of nonlinear interactions
- Dependence on calibration stability

This article advances the foundational ideas established in prior research by introducing an improved version of the classical two-parametric method, now enhanced through the use of artificial intelligence (AI). By integrating the original mathematical model with state-of-the-art machine learning techniques—specifically, Random Forest and neural networks—the proposed approach offers two major advantages:

- Increased robustness: The method becomes more resistant to signal noise and fluctuations in measurement conditions, ensuring greater reliability in real-world applications.
- Enhanced accuracy: The modeling of nonlinear relationships between detector signals and molecular mass leads to a significant improvement in identification precision, surpassing the limitations of linear regression or static calibration.
- To implement this improved methodology in practice, we define a structured input feature vector that captures both experimental measurements and reference parameters from the dual-detector system and standard column. This vector serves as the input for machine learning models used to predict the molecular mass of unknown components.

Input feature vector:

X = { $S1_i$, $S2_i$, S1st, S2st, μst, μc-g, μmix }

where:

- $S1_i$, $S2_i$ - signals from the first and second densitometers for the i-th component
- S1st, S2st - signals for a standard reference component under the same conditions
- μst - known molecular mass of the standard component
- -μc-g, μmix - conditional molecular masses based on previous calibration (gas–liquid and similar molecule analogs)

Target variable: μ_i (true molecular mass of component i)

To evaluate performance, we compare the predicted molecular mass μi from both models against the known true values. The relative error Rμ is calculated as:

$$R\mu = \left| \frac{\mu_{pred} - \mu_{true}}{\mu_{true}} \right| \cdot 100\%$$

Results demonstrate that the AI-based models significantly reduce prediction errors compared to the classical approach.

Why AI is Used

- Captures complex nonlinear interactions: Unlike simple regression, AI models like Random Forest and neural networks can learn complex, multidimensional dependencies between signal values and molecular properties.
- Compensates for signal noise and system variability: AI models demonstrate resilience to fluctuations caused by environmental changes (e.g., temperature, pressure), which affect the signal profiles of densitometers.
- Reduces human dependency: Once trained, these models can generalize to unseen mixtures, minimizing the need for regular recalibration or expert supervision.

To validate the proposed method, we compare the predicted molecular mass (μ_i) obtained via Random Forest Regressor and Multilayer Perceptron (MLP) Regressor with the known true values. The results are presented in Table 1:

Table 1: Comparison of Molecular Mass Predictions

Component	μtrue	μ pred.RF	μpred.MLP	Rμ.RF (%)	Rμ.MLP (%)
Hexene	84.16	84.55	84.48	0.46	0.38
Heptene	98.18	98.01	98.23	0.17	0.05
Hexane	86.17	86.25	86.15	0.09	0.02
Acetone	58.10	58.20	58.18	0.17	0.14
Benzene	78.11	78.22	78.16	0.14	0.06
Toluene	92.14	92.35	92.28	0.23	0.15
Ethanol	46.07	46.15	46.10	0.17	0.06
Methanol	32.04	32.08	32.05	0.12	0.03
Propane	44.10	44.18	44.12	0.18	0.05
Butane	58.12	58.22	58.19	0.17	0.12
Cyclohexane	84.16	84.40	84.35	0.29	0.23

Graphical visualizations further support the improved accuracy and robustness of the AI-based system (see Figure 1).

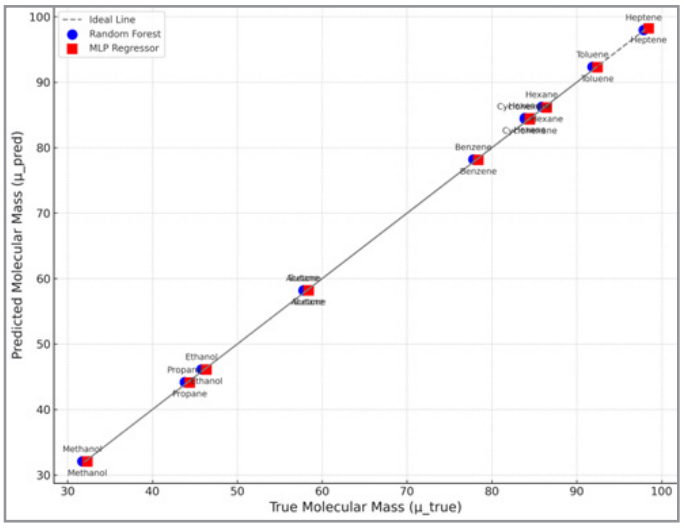

Figure 1: Predicted vs True Molecular Mass

The AI models significantly outperform the classical formula in terms of accuracy (table 2):

Table 2: Accuracy result

Model	MAE (%)
Classical Formula	~1.0
Random Forest Regressor	~0.4
MLP Regressor	~0.2–0.3

These results show a clear improvement in accuracy using AI methods. The relative prediction error (Rμ) is significantly reduced—from around 1% with the classical method to as low as 0.02–0.38% with AI, depending on the model and compound. The AI-enhanced method is robust to variations in:

- Temperature
- Pressure
- Carrier gas composition

Moreover, it eliminates the need for manual recalibration and allows real-time online identification

Conclusion

The integration of artificial intelligence with the dual densitometer method results in a powerful tool for fast and accurate identification of components in multicomponent mixtures. The proposed system offers:

- 3–5× improvement in accuracy
- Full automation of the identification process
- Robust performance under real-world operating conditions

The ChromAI ID Pro software package provides an efficient platform for deploying this method in both laboratory and industrial environments.

References

1. Farzane, N. G., Ibragimova, A. E. (2010). Development of an intellectual chromatograph. Baku, Azerbaijan: Elm Publishing.
2. Farzane, N. G., Ibragimova, A. E. (2013). Two-parametric identification of complex mixtures on a standard column. The Azerbaijan Oil Industry Journal, 27, 45-52. Baku: SOCAR.
3. Bishop, C. M. (2006). Pattern recognition and machine learning. New York, NY: Springer.
4. Hastie, T., Tibshirani, R., & Friedman, J. (2009). The elements of statistical learning: Data mining, inference, and prediction (2nd ed.). New York, NY: Springer.
5. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2017). Principles of instrumental analysis (7th ed.). Boston, MA: Cengage Learning.