Supplementary Information (SI) for Journal of Analytical Atomic Spectrometry.

In-Situ Multi-Element Soil Analysis Using Laser-Induced Breakdown Spectroscopy(LIBS)†

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1. Sample preparation

Soil samples were prepared using the tablet pressing method: the prepared sample was placed in an aluminum cup, with boric acid added as a supporting and protective medium (using a specialized fixture for the operation). Subsequently, a hydraulic press was employed to compress the sample into uniform cylindrical pellets (Fig. S1). The pressing pressure was set to 10 tons for dry samples and 30 kg for moist samples to prevent moisture loss during the compression process. The advantage of this method is that the samples are relatively dense, with good consistency between samples, resulting in high experimental reproducibility.

Fig.S1 shows some of the samples prepared using the pressing method.

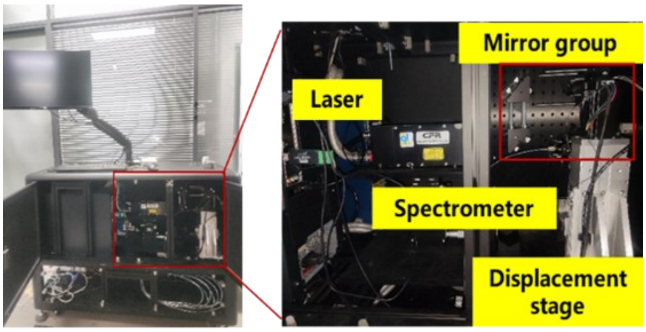


Fig.S2. LIBS System diagram

2. Variation trend of soil moisture content

Due to the influence of external environmental factors during the experiment, the moisture content of the samples changes over time. Therefore, the prepared samples must be analyzed immediately. Understanding the trend of moisture content changes in the laboratory helps guide the timing of sampling and analysis processes. To this end, under controlled laboratory conditions (temperature 23°C, humidity 30%), we monitored the moisture content trends of soil samples with different initial moisture levels at 2-minute intervals over a 12-minute period using the gravimetric method. As shown in Fig.S2, the horizontal axis represents the elapsed time since sample preparation, and the vertical axis shows the change in moisture content. The red vertical dashed line in the figure indicates that, to ensure the change in moisture content does not exceed 2% during the experiment, the entire process from sample preparation to analysis must be completed within 8 minutes to meet experimental precision requirements.

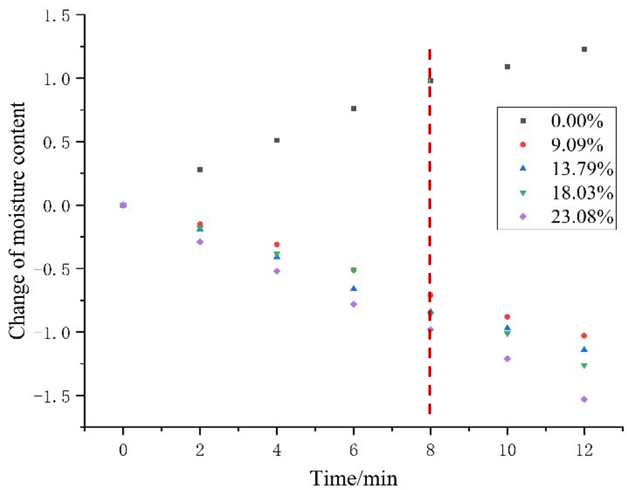


Fig.S3. Trends in soil water content under laboratory conditions

3. Correction model of ablation factor

To ensure the representativeness of the established model, characteristic spectral bands of elements such as carbon, hydrogen, oxygen, nitrogen, aluminum, calcium, magnesium, sodium, and potassium, along with 64 spectral lines selected by RF associated with Zn, Cr, Cu, and Pb concentrations, were chosen as the correction data. The reduction factors for each spectral band under varying moisture content conditions were calculated according to Equation 3 and subjected to exponential fitting. The correlation coefficient reached 0.998, indicating a strong correlation between the ablation factor and moisture content. The experimentally derived fitting function was incorporated into the ablation factor calculation formula, resulting in an explicit expression for the ablation factor.

$$\theta = \frac{1-\varepsilon}{0.074e^{(16.77\varepsilon)}+1.926} \tag{1}$$

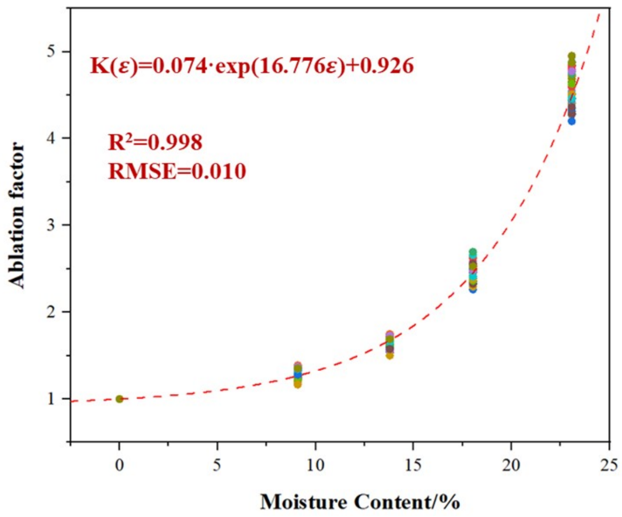


Fig.S4. Fitting result of reduction factor.

4. software interface

To facilitate practical application, this study developed a standalone software tool based on Python 3.8 and the PyQt5 module, which integrates and encapsulates the complete workflow described in the paper, including spectral preprocessing, moisture content analysis, the ablation factor correction model, multi-element quantitative prediction, and result analysis. The standard sample data only need to be processed once for model training and correction.

Fig.S5. Software interface.

5. Ablation Test

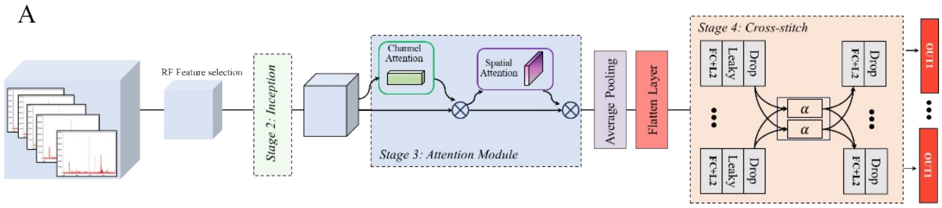
To validate the necessity of each complex module in MT-CAN and avoid arbitrary stacking of architectural components, we conducted systematic ablation experiments to evaluate the actual contribution of each component in addressing specific problems. Seven ablation models were defined: Model A (without residual connections), Model

B (without multi-branch Inception-like blocks), Model C (without attention mechanisms), Model D (without CrossStitch units), Model E (retaining only residual and attention modules), Model F (retaining only residual and CrossStitch modules), and Model G (retaining only attention and CrossStitch modules). By comparing the RMSE, as shown in Table 2. values of these models in elemental concentration prediction tasks, we further clarified the effectiveness and complementary relationships of each module across different task scenarios.

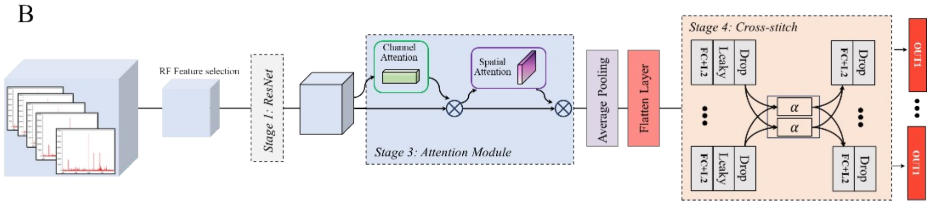
Table S1 RMSE of different models

Model	Zn	Cr	Cu	Pb	$R\bar{M}SE$
A	5.47	5.01	2.16	2.47	3.78
B	6.53	4.28	2.17	3.84	4.21
C	6.91	5.23	4.42	3.11	4.92
D	5.38	5.27	3.10	3.21	4.24
E	5.36	4.01	1.91	3.22	3.63
F	5.36	3.93	2.18	3.04	3.78
G	5.29	3.71	1.92	2.57	3.37

A



B



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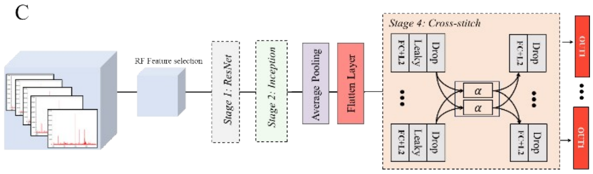

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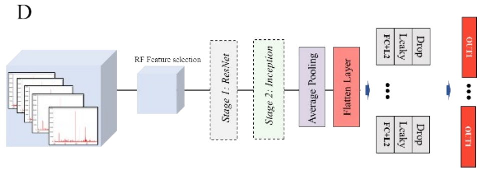
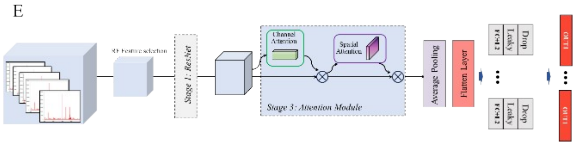
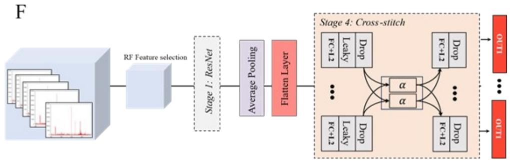


E



F



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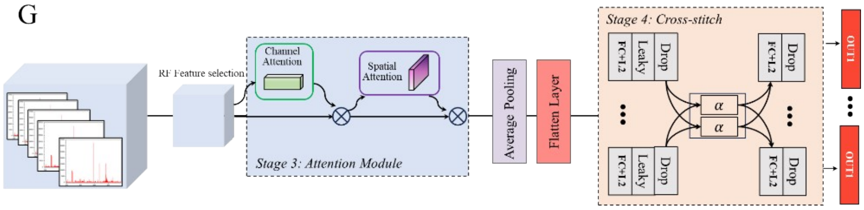

Fig.S6 Schematic diagram of the structure of different models