Development of an AI-augmented and smartphone-based handheld Raman spectrometer

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INTRODUCTION

The rapid detection and classification of jet fuel contaminants is crucial for private, commercial, and government aviation applications. Current methods typically rely on benchtop analytical techniques, which are unable to deliver timely results. While handheld Raman spectrometers offer quick qualitative analysis, the non-chemist end users often find it challenging to make decisions based on the spectrum collected in the field.

This project aims to develop an AI-augmented and smartphone-based Raman spectrometer designed to be an affordable and effective alternative to existing benchtop and field-testing methods. By incorporating AI, the system can be deployed in the field to detect and report jet fuel contaminants, such as hydraulic fluids, which may be phosphate ester, mineral, or polyalphaolefin (PAO)-based.

MATERIALS & METHODS

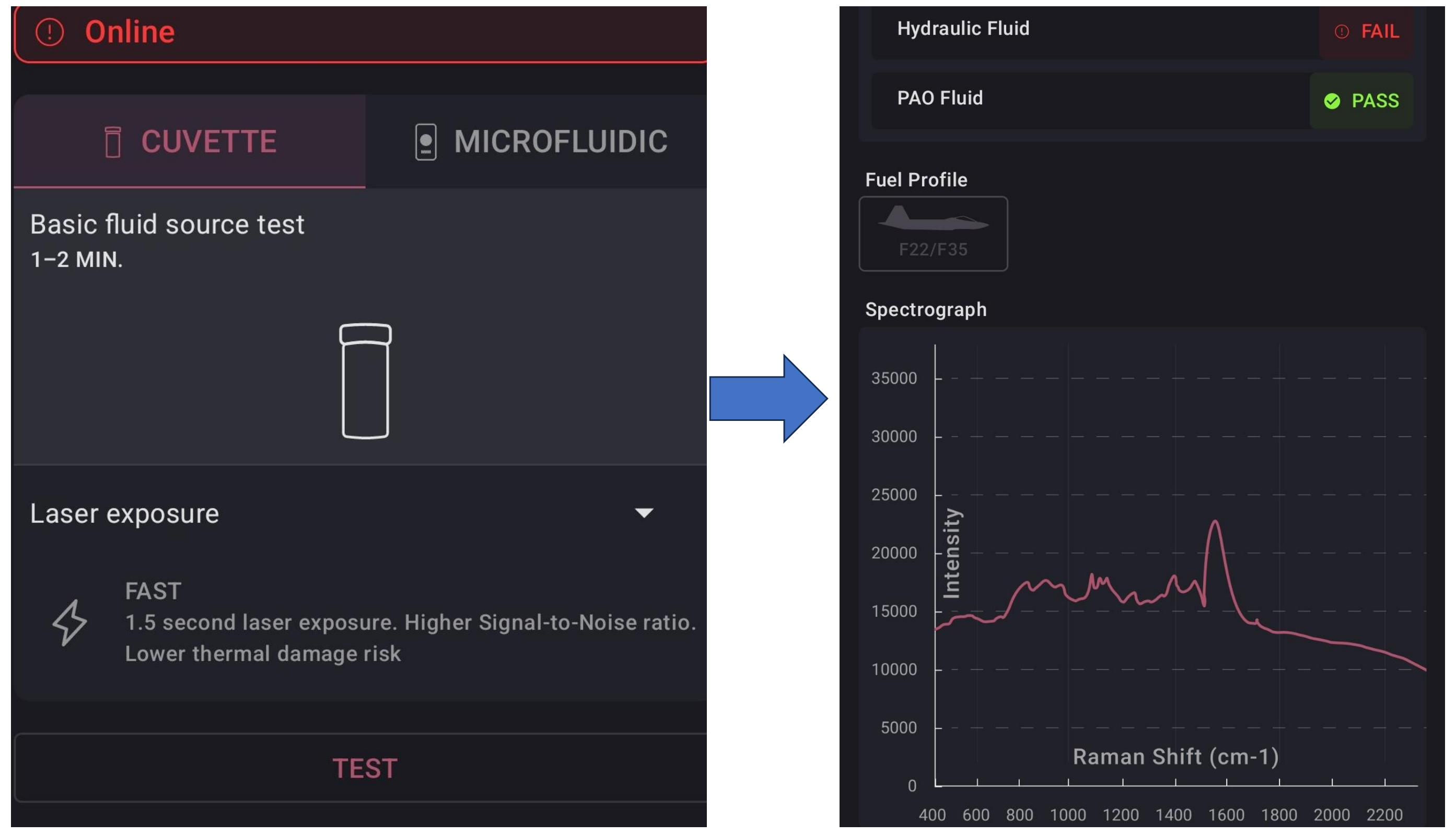
Five different jet-A fuels have been used in this study. Six different aviation hydraulic fluids, three synthetic-, two petroleum-, and one phosphate ester-based, were used as simulated contaminants. In total, 150 unique samples, each with replicates, were created from spiking hydraulic fluids in jet fuel at concentrations ranging from 1% to 0.0625% (v/v). Over 15,000 spectra were collected from neat and contaminated samples for training and testing the AI model.

A handheld Raman spectrometer (HandyRam, Field Forensic Inc., St. Petersburg, FL, USA) with a 785 nm laser was employed for spectral collection. The samples were placed in 2 mL amber vials for analysis in the instrument's vial compartment. The integration time of 5.0 seconds for each spectrum was determined by the autointegration feature. Automatic baselining was not used during data collection. The spectral range was recorded from 400 to 2300 cm^{-1} at 1 cm^{-1} intervals. Spectral data acquisition was performed using the Peak software (V1.01.0068, Snowy Range Instruments, Wyoming, USA).

RESULTS & DISCUSSION

Thus far, the AI model has correctly categorized 96% of samples it has been tested on. The extent to which it could quantize contaminants, or precisely categorize samples based on the specific contaminant, is unknown because the model is only programmed to identify the presence or lack of a contaminant since the purpose is to provide a quick answer for non-chemist field users.

Part of the user-interface for the proposed spectrometer, which is under continued development, is shown below in **Figure 1**. **Figure 2** is a 3D rendered image representing a prototype model of the proposed spectrometer.



Basic fluid source test
1–2 MIN.

Laser exposure

FAST
1.5 second laser exposure. Higher Signal-to-Noise ratio. Lower thermal damage risk

Hydraulic Fluid: FAIL

PAO Fluid: PASS

Figure 1. Partial user interface for the proposed spectrometer. The user is prompted to choose between basic or microfluidic-enhanced analysis. Once the spectrum has been generated, the system will display the spectrum and report a determination on the presence of absence of target contaminants.

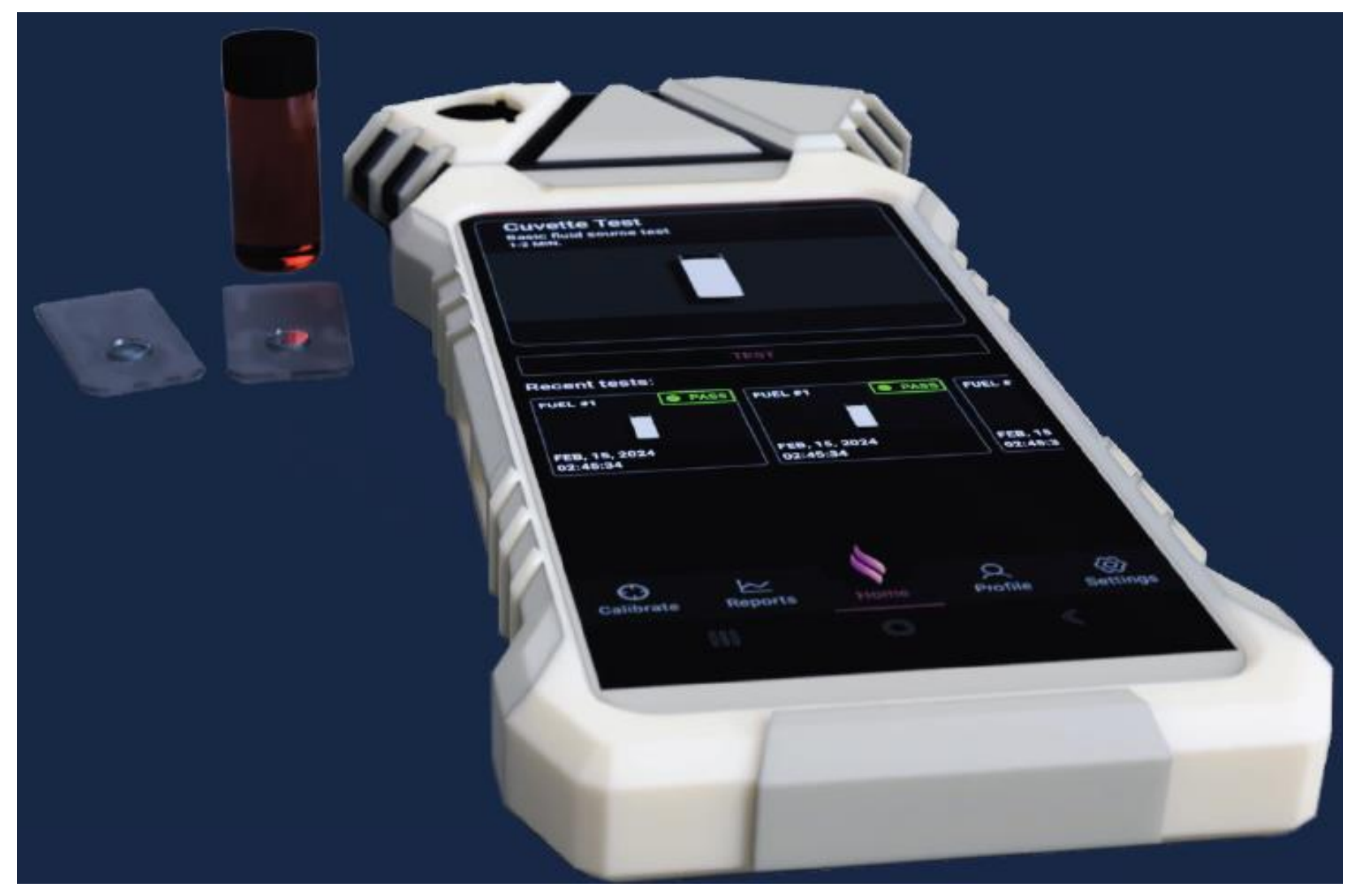


Figure 2. 3D rendered image of the Blaise prototype.

CONCLUSIONS AND FUTURE WORK

The present work investigated jet fuel contamination as an end use. Handheld Raman spectroscopy has been applied in many disciplines including forensics[1], medicine[2], art[3], and even geology[4]. We envisioned to develop an inexpensive handheld Raman spectrometer that uses deep learning AI tools to rapidly interpret spectra on the behalf of the end-user in the field. Because the lower-limit of detection required for real-world application is much lower than 0.0625% (v/v), approximately equivalent to 625 ppm, the application of SERS (Surface Enhanced Raman Scattering), potentially in combination with other microfluidic technology, will be investigated in future work to improve the sensitivity of the spectrometer. Future work will investigate these applications with varied approaches to account for the unique challenges brought about by different sample types.

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MATERIALS & METHODS

Table 1 below contains information regarding each hydraulic fluid contaminant.

Table 1. Classifications and additional information for the six hydraulic fluids used in this work.

Hydraulic Fluid	Classification	Additional
MIL-PRF-87257C	Synthetic	-
HyJet IV-A	Synthetic	Phosphate Ester-Based
MIL-PRF-87252C	Synthetic	Contains PAO additives
MIL-PRF-83282D	Synthetic	Contains PAO additives
MIL-PRF-5606H	Petroleum	Mineral oil-based
MIL-PRF-5606J	Petroleum	Mineral oil-based

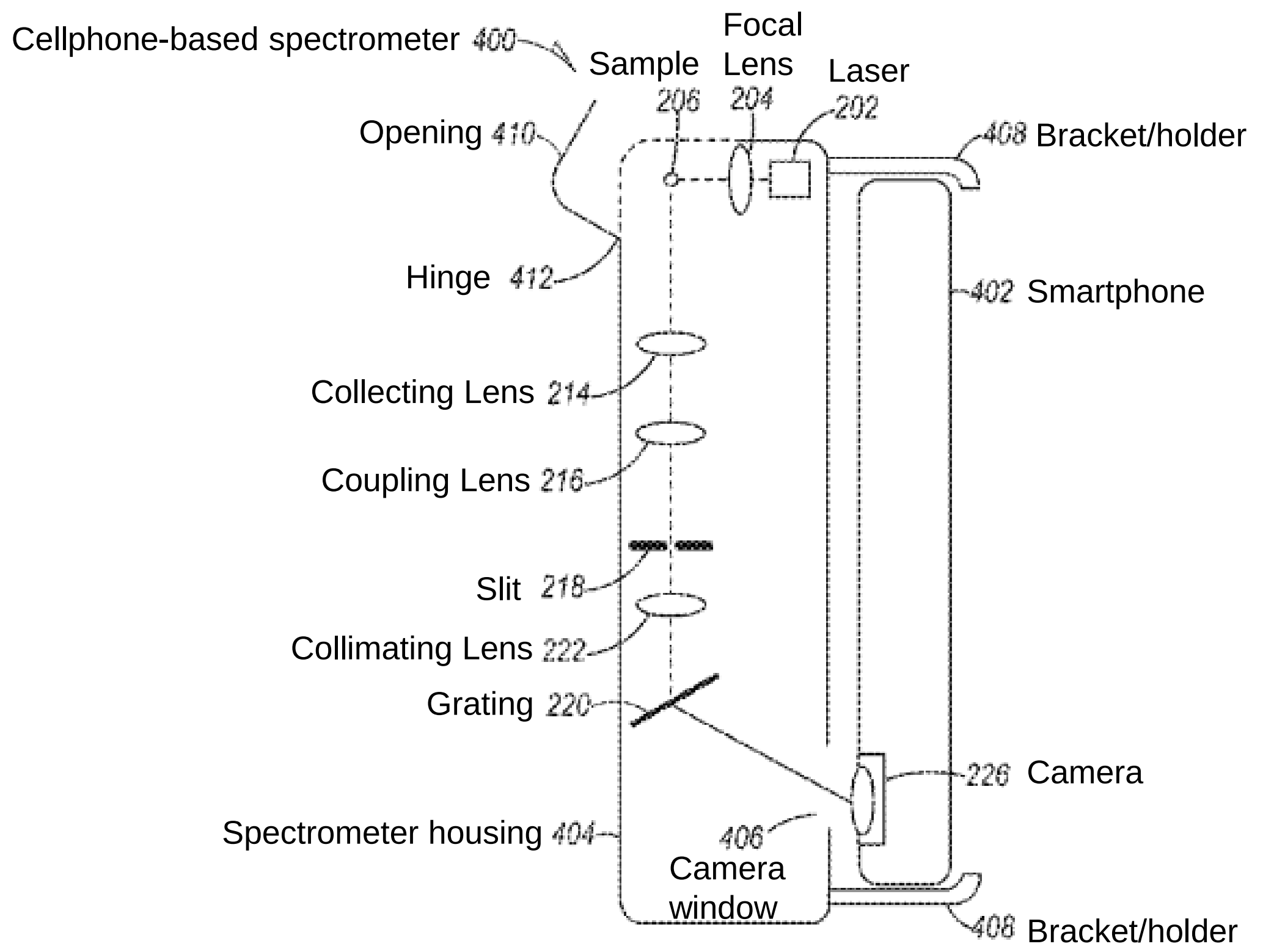

Figure 2[5]. Original Texas A&M prototype.

In January 2024, Texas A&M invented a patent for a cellphone-based Raman spectrometer[5]. **Figure 2** above shows the proposed design from the patent. The patent was later acquired by Forward Edge-AI, and it served as a starting concept for the handheld spectrometer under development in the current work. The physical spectrometer device is being developed in parallel with the AI model. The model is tasked with binary classification: it reports samples as either contaminated or uncontaminated.

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