Optical Chemiluminescence Diagnostics for Syngas Composition and Combustion State

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Abstract

This note proposes a non-intrusive optical method for assessing syngas composition and combustion quality using flame chemiluminescence. By observing emission from excited radicals (OH*, CH*, and C_2), it is possible to infer air–fuel ratio, combustion stability, and the presence of carbon-rich species. The approach is intended as a fast, low-cost diagnostic layer rather than a replacement for conventional gas analysis. The concept is well suited to structured investigation as a PhD topic.

1. Motivation

Syngas composition varies significantly depending on feedstock and gasifier conditions, typically comprising mixtures of H_2, CO, CH_4, CO_2, and N_2. Conventional measurement techniques (e.g. NDIR, TCD, lambda probes) are often:

- intrusive or require gas sampling,
- relatively slow,
- costly in industrial environments.

There is therefore value in a real-time, in-situ diagnostic method based on combustion behaviour.

2. Principle

During combustion, short-lived excited radicals emit light at characteristic wavelengths:

Species	**Wavelength**	**Interpretation**
OH*	∼310 nm	Oxidation zone / flame front
CH*	∼430 nm	Hydrocarbon breakdown
C_2 (Swan bands)	∼516 nm	C–C chemistry / soot precursors

These emissions arise from reaction-kinetics/flame-chemistry rather than bulk temperature alone, making them sensitive to both mixture and fuel composition.

3. Core Measurement Concept

The approach is based on measuring intensity ratios:

$$R_1 = \frac{\mathrm{OH}^*}{\mathrm{CH}^*} \quad \text{(air–fuel ratio)} \tag{1}$$

$$R_2 = \frac{\mathrm{C}_2^*}{\mathrm{CH}^*} \quad \text{(hydrocarbon richness)} \tag{2}$$

$$R_3 = \frac{\mathrm{C}_2^*}{\mathrm{OH}^*} \quad \text{(soot tendency)} \tag{3}$$

In addition, temporal behaviour provides diagnostic information:

- Standard deviation of OH* intensity → flame stability
- Cross-correlation between bands → regime transitions

4. Role of C_2 Chemiluminescence

The inclusion of C_2 (Swan bands) is key to extending the method beyond conventional OH*/CH* sensing.

4.1 Physical Significance

C_2 emission is associated with:

- presence of C–C bonds,
- locally fuel-rich regions,
- formation of soot precursors.

4.2 Diagnostic Value

Condition	OH	CH	C_2	**Interpretation**
H_2-rich gas	High	Low	≈0	Clean combustion
CO/H_2 mix	Moderate	Low	≈0	Typical syngas
CH_4 present	Moderate	High	Low–mod	Methane content
Heavy HC / tar	Lower	High	High	Soot risk / contamination

Thus, C_2 provides sensitivity to carbon chemistry and enables discrimination between different syngas compositions.

5. Additional Spectral Features

Other emissions of potential interest include:

- CN bands (∼388 nm): nitrogen-containing species
- Na/K lines (∼589 nm): contaminants or ash
- Continuum emission: soot radiation and incomplete combustion

A multi-band or spectrally resolved approach may allow further discrimination using statistical or machine learning techniques.

6. Implementation

A practical system could consist of:

- Photodiodes with narrow bandpass filters (310 nm, 430 nm, 516 nm)
- Transimpedance amplifiers (TIA front-end)
- ADC and embedded processing (e.g. STM32 class device)

Signal processing would include averaging, ratio calculation, and temporal analysis.

7. Applications

Potential applications include:

- Gasifier monitoring
- Industrial burner optimisation
- Detection of:
  - flame instability,
  - soot formation,
  - poor mixing or fuel variation,
  - calorific output of the current syn gas

8. Research Opportunity

Key open questions suitable for PhD investigation include:

- Calibration of optical signals against known gas compositions
- Sensitivity to temperature and pressure variations
- Robustness under optical fouling
- Extension to spectrally resolved measurement

9. Conclusion

Multi-band chemiluminescence sensing offers a promising route to fast, non-intrusive diagnostics for syngas combustion. The addition of C_2 emission provides a potentially valuable link to fuel composition, extending the method beyond simple air–fuel ratio measurement. The concept warrants structured experimental validation and is well suited to academic–industrial collaboration.