Uses of gas analysis/chemometrics in relation to health.

**(intro + Why gas analysis)**

Identification of constituent molecules of gasses is vital in practical applications such as medical diagnostics [HORVATH REF] and environmental monitoring[MORE WITH SOURCES]. For medical diagnostics the general goal is to diagnose diseases with greater accuracy and ease. Many different ways of diagnosing the human body are available such as by blood sample or imaging techniques. An upcoming branch of diagnosis is that by analysis of human breath. Breath analysis has the benefit of being nonintrusive, thereby being much more easily implemented by medical professionals as nonintrusive medical instruments undergo less strict control by regulatory parties like the FDA and EMA.

**(How gas analysis)**

Diagnosis by way of breath is performed by analysing metabolic molecules which diffuse from the bloodstream into the lungs and breath. Concentrations of these molecules result from certain chemical processes within the body, and as these chemical processes can be related back to diseases and general metabolism, the study of breath can be used as a diagnostic tool.

**(why QCL spectroscopy and intro to rest of paper)**

One of the most common currently used techniques for gas analysis is gas chromatography – mass spectrometry (GC-MS). Although GC-MS achieves high accuracy, it has certain limitations. GC-MS is a specific test, meaning it requires knowledge of what to test for beforehand[REF to Zhe Hou paper]. This means it is limited in use to only cases where symptoms are already showing, and thus requires pre-diagnosis. GC-MS also requires sample preparation, limiting its use to trained professionals. [WHAT ARE THE PROS/CONS OF THE OTHER SPECTROSCOPY METHODS MENTIONED BY ADONIS? December 15 paper on diabetes and QCL] A gas analysis method using a quantum cascade laser for spectroscopy is treated in this paper. When properly developed this form of analysis should need little preparation and therefore be more easily accessible. A priori knowledge of what molecules to test for is also not necessary for the measurement itself, which makes it a promising tool for laying statistical relations between concentrations of molecules and the health status of individuals.

**(Background to the research)**

A spectroscopy setup using a quantum cascade laser (QCL) is described and the subsequent data processing is extensively treated. The setup is made and extensively treated by A. Reyes Reyes as his PhD project funded by Fundamenteel Onderzoek Materie (FOM) foundation[REF to his papers]. Z. Hou worked on the setup under supervision of A. Reyes Reyes and has also treated it extensively[REF to masters paper]. Measurements processed in this research are from breath samples of 35 healthy volunteers, and 35 asthmatic volunteers. These samples are from children from the Sophia Children’s hospital in Rotterdam, all with their and/or their parents’ informed consent. The goal of this work is twofold. Firstly to decrease the uncertainties with which the compounds and its concentrations are determined. Secondly the goal is to find a reliable way of distinguishing and identifying breath of healthy and asthmatic children by way of the compounds present and their concentrations.

**(“ how QCL spectroscopy” is for next chapter, where the setup and its underlying measurement theory is explained)**