

# Sunset-calc: An R Shiny Application for Processing Thermo-Optical Analysis Data from Atmospheric Aerosol Measurements



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### **INTRODUCTION**

- > Atmospheric aerosols have adverse effects on human health1
- ➤ Atmospheric aerosols are emitted from natural and anthropogenic sources²
- $\triangleright$  Radiocarbon (<sup>14</sup>C) is a naturally occurring radioactive ( $t_{1/2}$  = 5730 years) isotope constantly formed in the upper atmosphere
- ➤ Source apportionment with <sup>14</sup>C can unequivocally separate biogenic from fossil-fuel derived sources
- Thermal-optical analysis aims to separate non-refractory organic carbon (OC) from refractory elemental carbon (EC)

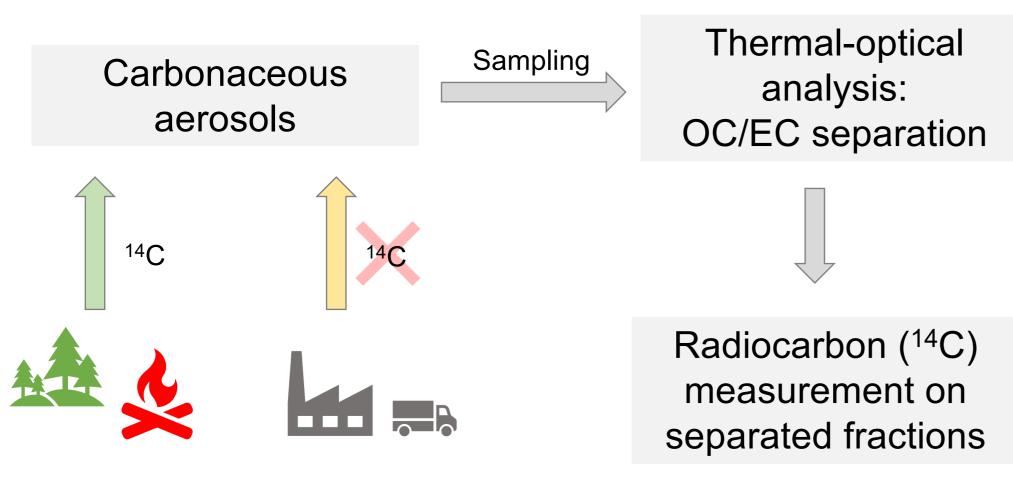
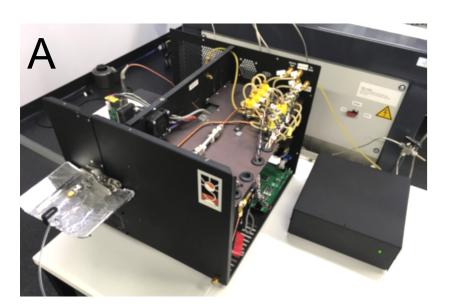


Fig. 1: From aerosol emissions to a radiocarbon measurement. Aerosols from biogenic emissions and biomass combustion processes contain <sup>14</sup>C, whereas aerosols from fossil-fuel combustion are completely devoid of <sup>14</sup>C. Thermal-optical analysis separates organic carbon (OC) from elemental carbon (EC) before radiocarbon measurement.

## **METHOD**

- A Sunset thermal-optical analyser is used for the physical separation of OC and EC
- The OC/EC separation is monitored by a laser and a non-dispersive infrared (NDIR) detector



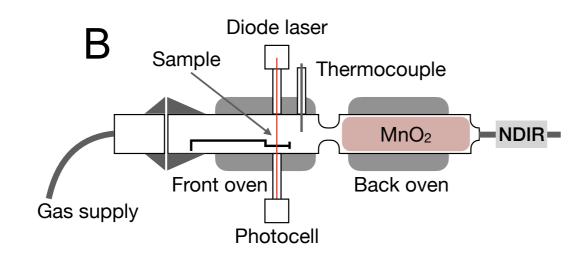


Fig. 2: Thermal-optical analyser. A: Sunset OC/EC analyser with non-dispersive infrared (NDIR) detector on the right. B: Scheme of the sample oven in the Sunset OC/EC analyser with a laser for OC/EC separation monitoring.

- Some OC is converted into EC (charring)
- Some EC is lost, which leads to a reduced EC yield
- Charring and EC yield must be optimised using the temperature for each aerosol filter campaign
- These artefacts must be corrected for
- 800 S1 S2 S3 S4 40 Laser attenuation (A.U.)

  Charring EC loss

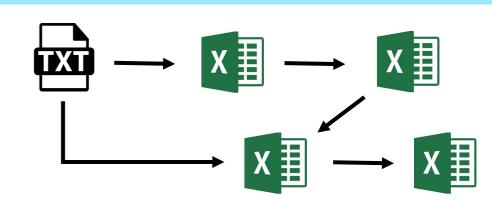
  EC loss

  Time (s)

Fig. 3: Thermal-optical analysis. Temperature and laser attenuation signal with a 4-step (S1 to S4) OC/EC separation protocol where S1 is pure OC and S4 is pure EC.

#### **GOAL AND MOTIVATION**

- Improve processing of thermal-optical analysis data
- Excel spreadsheets were previously used
- Analysis was time-consuming and complicated with compatibility issues and various template versions



**Fig. 4: Previous workflow.** Several Microsoft Excel spreadsheets were used for data analysis.

Caic

Fig. 5: Sunset-

calc logo.

## **RESULTS**

- Data analysis from spreadsheets was rewritten and extended in R
- R Shiny was used to build a web application
- > The Sunset-calc<sup>3</sup> application was deployed on an R server
- > Sunset-calc provided instant benefits:
  - > Calculation of EC yield and charring with visualisations
  - Corrected carbon amount calculation for custom protocols
  - ➤ Tedious & time-consuming spreadsheets replaced with drag and drop and almost instant results
  - > User and platform independent and with version control

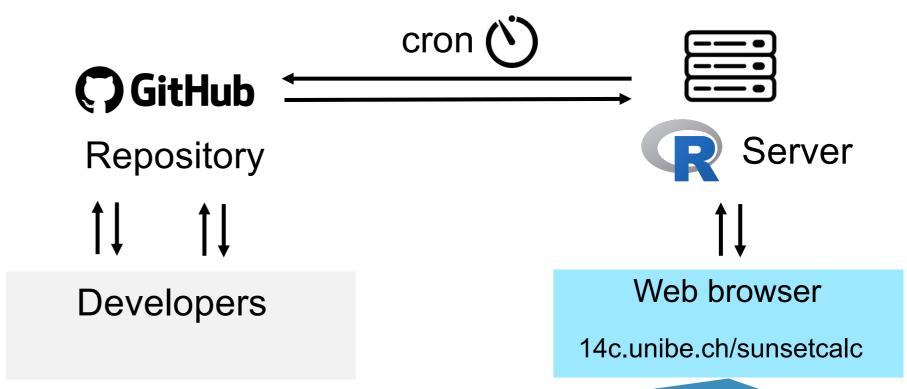




Fig. 6: Sunset-calc server deployment and user interface. The desired analysis is selected in the menu and the analyser raw data files are uploaded in the web interface. The calculation results are provided as a download. Changes to Sunset-calc in the repository are automatically deployed to the R server.

## CONCLUSION

- Sunset-calc simplified and streamlined the lab workflow with automated data evaluation
- > R with R Shiny provides a simple solution to create web applications suitable for people with little prior programming skills