

# Calculating Plant Isoprene from FIS Data

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1:50 PM

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2013\_05\_21  
Plant isopr...

The first sheet titled 2013\_05\_21 Plant isoprene amount from FIS data SEW.xlsx can be used to calculate the amount of isoprene being given off by a plant if a sample is taken from the sample exhaust of the LI-COR and injecting it into the FIS using a needle and syringe.



2013\_05\_28  
Calculatin...

When the LI-COR 6400 is connected directly to the FIS calculating isoprene amounts can be bit more tricky than simply making injections using a needle and syringe. The attached spread sheet titled 2013\_05\_28 Calculating Isoprene with FIS attached to LI-COR SEW.xlsx will calculate the average isoprene mole fraction (ppb) and the total amount of isoprene in nmol m<sup>-2</sup> over a given time period. The spread sheet automatically takes into account the integration time of the FIS (i.e. 0.1, 1, 5 s) and will subtract out background levels of isoprene. The user will need to provide the following information for the spreadsheet to work correctly

1. RAW data from the FIS (just the time and photon counts per second)
2. The calibration of the FIS: both the slope (counts / isoprene ppb) and the Y intercept (counts). The second sheet with the tab labeled "Calib" provides the calibration data analysis
3. The FIS total flow (sccm)
4. The FIS oxygen flow (sccm)
5. The LI-COR sample flow rate (μmol s<sup>-1</sup>)
6. The Leaf area in the LI-COR (cm<sup>2</sup>), this is usually 6 cm<sup>2</sup>
7. To subtract out background isoprene, the background isoprene level should be monitored for a minute or two. This can be done at any point in the experiment as long as the start and stop times of the background sampling period are recorded. If you do not wish to subtract out the background leave the start time blank in the isoprene background section and the Y intercept counts from the calibration will automatically be used instead.
8. The start and stop time of each sampling period to be analyzed.

Math

$$\text{Average Isoprene (ppb)} = \frac{\text{average counts} - \text{average background counts}}{\text{slope (counts isppb}^{-1})}$$

$$\text{Isoprene (nmol m}^{-2} \text{ s}^{-1}) = \frac{\text{counts} - \text{avg bkg counts} * 1e^{-9} \text{ nmol mol}^{-1} * 0.0446^{*3} \text{ mol L}^{-1} * \text{FIS sample flow rate}^{*4} \text{ L s}^{-1} * \text{LICOR flow}^{*6} \text{ mol s}^{-1}}{\text{slope}^{*7} \text{ counts isppb}^{-1} * \text{FIS sample flow rate}^{*8} \text{ mol s}^{-1} * \text{leaf area m}^{-2}}$$

Total Isoprene (nmol m<sup>-2</sup>)

$$= \frac{\text{total counts} - (\text{avg bkg counts} * \text{\# of samples}^{*1}) * 1e^{-9} \text{ nmol mol}^{-1} * 0.0446^{*3} \text{ mol L}^{-1} * \text{FIS sample flow rate}^{*4} \text{ L s}^{-1} * \text{integration time}^{*5} \text{ s} * \text{LICOR flow}^{*6} \text{ mol s}^{-1}}{\text{slope}^{*7} \text{ counts isppb}^{-1} * \text{FIS sample flow rate}^{*8} \text{ mol s}^{-1} * \text{leaf area m}^{-2}}$$

Explanation of Math

1. # of samples - This is the number of samples or readings recorded by the FIS during the user specified sample period. For example if you specified the start time to be 1 second and the stop time to be 5 seconds and the integration time was 0.1 second the number of samples recorded by the FIS during this time period would be 50. This allows the background to be subtracted out for the entire sampling period specified by the user
2. 1e<sup>-9</sup> - converts from ppb or nmol/mol to mol/mol
3. 0.0446 - converts from a mole fraction to a molarity i.e. there are 0.0446 moles of a gas in 1 liter at standard temperature and pressure
4. FIS sample flow rate - This is the actual rate of sample air being drawn into the FIS this is obtained by subtracting the oxygen flow rate from the total flow rate and converting from sccm or standard cubic centimeters per minute which is a ml per minute (at STP) to liters per minute. This is converted to liters per second by multiplying by 0.016667 min sec<sup>-1</sup>.
5. integration time - This is the integration time of the FIS. This is calculated by simply taking the first time period after 0 in the time column that the user cuts and pastes into this spread sheet from the text file output by the FIS
6. LICOR flow rate - Because the flow out of the LICOR must be greater than the flow into the FIS some isoprene is "lost" and must be accounted for. The sample flow out of the LICOR is calculated by taking the sample flow from the LICOR in μmol s<sup>-1</sup> and multiplying by 1e-6 to convert to mols per second. This correlates to the FIS sample flow rate in which is in the denominator
7. slope - from the FIS calibration this is the number of photon counts per ppb isoprene
8. FIS sample flow rate - Because the flow out of the LICOR must be greater than the flow into the FIS some isoprene is "lost" and must be accounted for. The flow is converted to moles s<sup>-1</sup> by multiplying by 0.016667 min s<sup>-1</sup>, 0.001 ccm L<sup>-1</sup>, and 0.0446 mol L<sup>-1</sup>. This is correlated to the LICOR sample flow rate in the numerator.