<u>Comment 1:</u> As the new software is able to process also conventional eddy covariance data, I would like to see some comparison between data processed with the new software and established EC post-processing softwares, e.g. EddyPro, EddyUH (Mammarella et al., 2016).

**Reply:** As suggested we have included a comparison using EddyPro. The software codes yield comparable results. The regressions for wT and wCO2 fluxes, for example, show R<sup>2</sup>s of 0.99 and 0.97, respectively, slopes are 0.95 and 1.02, respectively.

**Changes:** The revised manuscript now also includes the suggested comparison, which was included in the supplementary files (Chapter S2 and Figures S2 und S3).

<u>Comment 2:</u>Test site is challenging from micrometeorological point of view. How about including data from some more ideal measurement site to analysis?

Reply: We share the notion that flux measurements in urban areas might appear more complex at first sight, but would like to point out that most towers in areas exhibiting high reactive gas fluxes have site specific challenges (Foken et al., 2012; , Park et al., 2013, Rantala et al., 2016:). The definition of an ideal measurement site is therefore often difficult. For an urban location we would argue that the site is of low to intermediate complexity (ie. homogeneous footprint in the two main flux footprint corridors, flat terrain (valley bottom)). The advantage of the present dataset is that (1) we deal with well characterized anthropogenic tracers (e.g. aromatic compounds), and (2) the PTR-qTOF-MS instrument possesses enough sensitivity to capture carbon isotope fluxes (e.g. 13C Toluene). We see this as an essential added benefit to the evaluation presented here.

Comment 3: The equation (1) is not correct and I am not satisfied with how Eq. (2) is derived.

**Reply:** The equation already included some simplifications (ie <w>>0) as pointed out by the reviewer.

**Changes:** We modified the derivation as and included the complete derivation as suggested by Rinne.

<u>Comment 4:</u> The required response time of sensor for eddy covariance is stated in the manuscript to be on the order of 0.1 s. However, e.g. Rantala et al. (2014) have shown the response time of a quadrupole PTR-MS to be around 1.2 s. Furthermore, they showed that above forest this response time lead to flux underestimation ranging from below 10% in daytime, to about 20% during night. Thus, if the response time of the instrument is in that range, sampling output at higher frequency does not actually lead to better frequency

response. The response time of PTR-ToFMS used in the measurements to test the software is not stated in the paper. The statement on page 3, lines 5-6 "...is nowadays mostly used for instrumentation that can measure single compounds fast enough (e.g. 0.1 s)..." may be bit optimistic.

Reply: Thank you for this valuable comment - we fully agree with the reviewer that with regards to cospectral attenuation the response time of a sensor (rather than the output frequency) is one of the key parameters that may govern the high frequency loss of an eddy covariance system. This holds particularly for the data of the VOC EC system exemplarily used here for the demonstration of the capabilities of the innFLUX open source code. The response time of a PTR-MS system depends in first order on the exchange rate of the sample gas in the inner volume of the instrument, which is largely governed by the drift tube volume and the volumetric flow, and for sticky compounds, on the properties and area of wetted surfaces. In both regards small dead volumes, reduced surface areas, inert materials, low pressure and high temperature improve the response time. Since the introduction of the PTR-MS method in the 1990s the achievable response times had increasingly improved from ~0.8 s in 1999 (Karl et al 2001) and about 1 s in 2000 (Rinne et al 2001) to at least 0.1 s in 2001 (Karl et al. 2002) as a consequence of design improvements driven by the requirements of the EC technique. The PTR-Qi-TOF instrument here has a characteristic time constant of 0.08 s. It is indeed important to point out how the response time of a closed path analyzer (amongst other dampening effects) affects the cospectral attenuation and how the EC flux can be corrected for such high frequency losses.

Changes: We conducted a thorough analysis of the cospectral behavior of the VOC EC system described here based on Foken et al. (2012a) and Lee et al. (2004). The added Chapter S4 in the supplement now guides the reader how to derive a model cospectrum from quality checked individual half-hour cospectra (example in Figure S3). It shows how to determine transfer functions describing high frequency lossed due to sensor separation, sonic path averaging, sensor path averaging (PTR-MS response) and tube attenuation, and how these attenuations cause loss of cospectral density at high frequencies, thus underestimating the flux (Figure 7). The new Chapter 3.5 in the main text points out the cospectral information calculated and stored by innFLUX, mentions both the experimental approach and the theoretical approach for the correction of high frequency losses, gives the user guidance which approach might be more appropriate, and details the procedure (reference to Chapter S4 and Figure S3) and results (Figure 7 and Figure S4) of the cospectral analysis.

**Comment 5:** On page page 4, lines 4-6 the authors give an example of systematic error caused by disjunct sampling as 23%, with sampling interval D=60 s, integral time scale t=25 s, and flux averaging time T=300 s, based on equation by Lenschow et al. (1994). However, setting D=0.1s, i.e. typical conventional eddy covariance sampling frequency, leads to flux underestimation of 15%. Thus, more than half of the flux underestimation is not due to

disjunct sampling, but rather undersampling the low-frequency contribution by this very short (5 min) flux averaging period. Similarly, for other flux averaging periods shown most of the underestimation does not derive from disjunct sampling. Furthermore, for typical surface flux measurement averaging periods (30 min = 1800s), the underestimation with sampling interval of even as long as 3 min causes flux underestimation of less than 10%. The authors give a similarly misleading statement on page 12, lines 15-16.

**Reply:** We acknowledge that the numbers in the original manuscript represent the sum of systematic errors due to DEC and block averaging interval. Figure 4 shows that DEC intervals of about 100s for T=1800 s would lead to a 10% bias. The general conclusion is that at certain DEC intervals the block averaging interval needs to increase and problems due to non-stationarity might arise, when T becomes too large.

**Changes:** We clarified the issue of DEC errors and averaging periods in the revised manuscript

<u>Comment 6:</u> Sensor separation (Page 5, line 3) is usually smaller source to lag time than is the long sample tube in the case of closed path analyzers such as PTR-MS.

**Reply:** OK we added that a long sample tube is also a relevant parameter.

<u>Comment 7.</u> I got the impression that the software is not performing frequency corrections to fluxes using cospectral densities. One could also correct for high-frequency losses in DEC measurements, if system response time is known, e.g. by test-run by the same system with continuous sampling.

**Reply:** We acknowledge that high frequency losses can be accounted for by using empirical formulas (e.g. Horst et al., 1997) and adjusting these to real 10 Hz data. The code outputs all spectral information, so that the user can determine system response times from co-spectral comparison. The code is not automatically implementing a correction to the data, since we believe these things are instrument specific and really need to undergo thorough evaluation by the experimentalist. Depending on the nature of a particular dataset (e.g. how many spectra are available for averaging? Is it a DEC dataset? How high are fluxes?) the high frequency correction can either be calculated from the co-spectral data directly or has to be based on a-priori information (e.g. an estimation of damping timescales).

**Reply:** innFLUX calculates and stores cospectral information for the correction of cospectral attenuation. Which approach for such corrections is suitable or whether there exists a meaningful way for spectral corrections at all cannot be decided without further consideration of the user. The user must take into account measurement station geometry and operational parameters, distribution of sources and roughness elements as well as length and quality of the dataset for their decision whether and how to correct for cospectral loss of covariance. They have to validate the

respective assumptions of their approach (e.g. cospectral similarity of sensible heat flux and VOC flux; does the data set allow to come up with an adequate model spectrum? Are geometry and the operational parameters sufficiently well defined to determine all significant transfer functions?) for their specific data set, the measurement site as well as the setup and operation of the EC system and its sensors. We therefore believe the specific situation needs to undergo thorough evaluation by the experimentalist. We acknowledge that the reader needs guidance how to use the cospectral information provided by innFLUX. Thus we conducted a thorough analysis of the cospectral behavior of the VOC EC system described here based on Foken et al. (2012a) and now provide procedures and results in the manuscript.

**Changes:** See reply to comment 4 for details.