Response to Anonymous Referee #1

We thank the reviewers for their constructive and helpful suggestions. We have provided our responses to the reviewers' comments and believe that our manuscript is much improved as a result.

The main paper improvements are:

- The abstract was rewritten.
- The goal of the study is formulated more clearly.
- The number of sites for validation of GELCA is increased.
- Proofreading and grammar check performed.

The reviewer's specific comments (shown in blue) are addressed below.

Anonymous Referee #1

Received and published: 8 September 2015#1:

The manuscript by Belikov et al. presents the development of a new adjoint modeling system A-GELCA. The novelty of this tool is combining a Lagrangian back trajectory model with an Eulerian adjoint model. The authors provide background on issues related to inverse modeling of CO2, which seems to be the intended application of this tool. The model estimates for various configurations (different resolutions of the Eulerian component) are shown compared to CO2 measurements from seven stations in Siberia. This is followed by evaluation of the model via comparison to forward modeling sensitivities and the Lagrange equality. Lastly, the authors show comparisons of adjoint sensitivities for different model configurations, highlighting the information brought through the coupling of Lagrangian and Eulerian components. The tools presented here seem to perform adequately and will be of value for future application studies. My main criticism is a lack of detail in many places in the manuscript, particularly when covering some of the more essential and novel aspects of the model development (how the Eulerian and Lagrangian components were coupled, or how the adjoint code was developed). Further, the article needs much work on the grammar and writing. I believe it will be suitable for publication after addressing these and other issues outlined below.

Comments:

Scope: It seems like evaluation of the forward model is a substantial part of this work; as such, this should be included in the abstract and introduction as one of the aims of the article, and the title itself should reflect this scope.

The goal of this study is to present the development and evaluation of an Adjoint of the Global Eulerian–Lagrangian Coupled Atmospheric model (A-GELCA). Evaluation of the forward model is necessary to show the potential of the proposed method.

Abstract and throughout: it seems odd to refer to “development of the adjoint of a Lagrangian model”, since Lagrangian models are self adjoint by construction. So saying “Lagrangian adjoint” seems redundant.

Text in the paper was revised. “Lagrangian adjoint” is replaced with “Lagrangian component”

5984.17: this entire sentence is rather vague. Could the authors clarify, quantitatively, what is mean by “effective in reproducing”, “high uncertainty” and “low resolution”? Without any numbers, such statements have little context or impact.

The sentence revised as follows: “The forward simulation shows that the coupled model improves reproducing of the seasonal cycle and short-term variability of CO_2.”

However, we do not consider it is necessary to include any numbers in the introduction. More details were added to main part.

5985.13: Can the authors be any more specific than “a number of studies have proposed improvements” and then citing several papers? What are the improvements, and which are relevant to the topic of this work in terms of those related to resolution, or coupled Eulerian/Lagrangian frameworks?

Revised as follows:

“A number of studies have proposed improvements to the inverse methods of atmospheric transport, i.e. the efficient computation of the transport matrix by the model adjoint proposed by Kaminski et al. (1999b), use of monthly mean GLOBALVIEW-CO_2 ground-based data (current version is for 2014) by Rödenbeck et al. (2003), development an ensemble data assimilation method by Peters et al. (2005), flux inversion at high temporal (daily) and spatial (model grid) resolution using for the first time of continuous CO_2 measurements over Europe by Peylin et al. (2005), use satellite data to constrain the inversion of CO_2 by Chevallier et al. (2005), develop of a new observational screening technique by Maki et al. (2010).”

Paper by Kaminski et al. (1999b) is related to the adjoint. Paper by Chevallier et al. (2005) is related to use of satellite data. Flux inversion at high temporal (daily) and spatial (model grid) resolution using for the first time of continuous CO_2 measurements over Europe is discussed by Peylin et al. (2005).

Eulerian/Lagrangian frameworks is discussed later (5987.10-16): “In order to exploit the advantages of both methods, Lagrangian and Eulerian chemical transport models can be coupled to develop an adjoint, that is suitable for the simultaneous estimation of global and regional emissions. Coupling can be performed in several ways; e.g., a regional-scale LPDM can be coupled to a global Eulerian model at the domain boundary (Rödenbeck et al., 2009; Rigby et al., 2011), or a global-scale LPDM can be coupled to an Eulerian model at the time boundary (Koyama et al., 2011; Thompson and Stohl, 2014).”

5985.20: For recent measurement updates, a reference from 1999 doesn’t seem very recent.

Replaced with (Karion et al., 2013; Tohjima et al., 2015)

5986.16: It would take a prohibitively large number of forward model evaluations to evaluate such a matrix for an inversion with the same resolution of an adjoint-based approach.

Revised as: "Theoretically, to compute such matrix the transport model is run multiple times with set of prescribed surface fluxes. However, this would require an extremely large number of forward model evaluations. The adjoint of the transport model is an efficient way to accelerate calculation of concentration gradient of the simulated tracer at observational locations (Kaminski et al., 1999)."

5986.24: "Recent studies. . ." It seems odd to switch the discussion here to CO, given the previous focus on long-lived tracers, CO2 in particular. Why not instead cite/discuss the set of current studies using adjoint models to invert satellite CO2 data? I believe there are several.

Revised as follows: "Recent studies have used this method to constrain estimates of the emissions of CO_2 using retrieved column integrals from the GOSAT satellite (Basu et al., 2013; Deng et al., 2014; Liu et al., 2015)."

5986.28: ". . .speeds the process of inverse modeling" is only true for high dimensional systems.

In 5985.23-30 we stated: "The satellite observation data from current (GOSAT, Kuze et al., 2009; Yokota et al., 2009; OCO-2, Crisp et al., 2004) and future missions (CarbonSat/CarbonSat Constellation; Bovensmann et al., 2010; Buchwitz et al., 2013) offer enormous potential for CO_2 inverse modeling. Optimal application of large observed datasets requires expanding the inverse analysis of CO_2 to finer resolution, higher precision and faster performance." A large number of observations and resolution of the considered model indicate that the existing and developing inverse modeling system can be attributed to the high dimensional systems.

5988.20: The background. . ." I didn't really understand what was being said here or how the modeling setup works in this regards.

Here "The background grid values of the concentrations" are the concentrations calculated by Eulerian model.

To clarify the sentences about the model setup we revised section 2.1.

5989.3: The description of the coupling of the eulerian adjoint model with the Lagrangian model is rather vague. This statement, that it was coupled at the "time boundary" is made a few times, but to be honest I don't really know what it means. Given that (a) this coupling is the single most unique and exciting feature of the A-GELCA model and (b) articles in GMD are for the expressed purpose of describing algorithmic model details, this should clarified in further detail, at the level of making the process understandable and reproducible by a reader.

We revised section 2.1 and added short descriptions of coupling procedure to the text to clarify the sentences about the time boundary coupling: "The scheme of concentration calculation for the given location includes coupling of two model approaches. NIES TM calculates global concentrations for the selected time period (usually 1 year to exclude spin-up effect), but stops 7 days before the time of the observations. To obtain the concentrations for the observation time we transport the background concentrations from NIES TM gridbox to the location of observation point along the trajectory ensemble calculated by FLEXPART model and add contribution from surface sources. Therefore we have implemented the coupling at a time boundary in the global domain of the NIES transport model, while nested regional modeling systems such as one by Rodenbeck et al (2009) have to couple at both region boundary and time boundary."

Here we just repeat the main features of the coupling. Detailed information may be found in original paper by Ganshin et al. (2012).

5989.25: "performs well" is very vague. Can the authors be more specific?

The text is revised as follows: "To ensure that this is the case, the NIES TM model has been evaluated extensively. Comparisons against SF_6 and CO_2 (Belikov et al., 2011, 2013b), CH_4 (Patra et al., 2011; Belikov et al., 2013b), and ^{222}Rn (Belikov et al., 2013a) measurements show the model ability to reproduce seasonal variations, interhemispheric gradient and vertical profiles of tracers." For details please check papers shown above.

5992.5: Is it that the errors are unbiased or that the background estimate itself is unbiased?

Here it is assumed, the model simulations are unbiased. Observations are unbiased normally.

5992.6: This capital bold H applied as a matrix is already linear by definition. If the authors intended to more generally describe a potentially nonlinear forward model operator, they should use capital cursive H.

Revised as follows: "Equation 2 has an analytic solution …"

Did the authors also generate/evaluate a tangent linear model? If not, what is there intended path towards deriving an inverse modeling system (many formulations of which require a tangent linear model, i.e., incremental 4D-Var with CG optimization, etc)? Or will their system only worth with optimization approaches such as using the BFGS variable-metric quasi-newton algorithm?

Yes, we constructed tangent linear model. We stated "The tangent linear and adjoint components of the Eulerian model …" at 5984.7, 5994.1, 5999.22.

5993.11: Previously (5992.24) a 1x1 scale was referred to as low resolution, but here 1x1 is used for the "high resolution" FLEXPART runs. This is a bit inconsistent. I was expecting FLEXPART simulations to be run at a much finer (i.e. 10's of km) scale.

At line 5992.24 the sentence "standard low-resolution" replaced with "standard resolution".

Currently we have no meteorological data suitable to run the FLEXPART model with higher resolution (i.e. 0.5 degree). However, use a model with resolution of 1x1 degree for flux inversion is normal now.

The set of measurements used for evaluation (7 sites) seems pretty thin compared to the amount of available CO2 measurements available. The NOAA GMD network alone has more than 100 measurement sites. Now, perhaps forward model evaluation isn't a goal of this work (see previous discussion, this wasn't clear), but if it is then it should be done more comprehensively.

Number of sites for validation of GELCA is increased. Section 4 was revised.

5994.7: "We recognize. . . is quite problematic" I didn't understand the point that the authors are trying to make here. Can they reword?

Reworded: "We recognize that is quite problematic to use the highly uncertain surface fluxes to simulate the tracer concentrations and use these concentrations for estimating the quality of different model configurations. Nevertheless, we cannot improve our analysis, because we do not have concentration measurements for tracers whose surface fluxes are more accurately known, like SF6."

5994.22: I recognize that there are continuous vs discrete approaches for developing adjoint models, that there are benefits/drawbacks to each approach, and that the authors

have adopted the discrete approach for specific reasons. But is it fair to only here mention the benefits of this approach, and none of the drawbacks?

We added "The main drawback of the method is that the deriving of discrete adjoint of Eulerian model is a significant technical challenge."

5996: For the forward model sensitivity, use lambda_F throughout, not just in equation 5.

Revised accordantly.

5996.14: Why is a perturbation needed for an adjoint simulation? Do you mean forcing? Or that the cost function was defined to be 1 ppm per grid cell?

There was misprint in this section.

The text was revised, as: "In the first test, adjoint simulations were carried out using an initial CO_2 distribution, zero surface flux for 2 days (1-2 January 2010) and a horizontal grid with resolution 2.5° × 2.5°. The adjoint gradient was then compared with that from the finite difference calculated using Eq. (3). This equation was selected in order to save CPU time by minimizing the number of forward model function calculations. For this test we used $\varepsilon = 0.01$."

Section 3: I recognize that the long-term goal is inverse modeling. However, the application and testing of the model thus far is just for sensitivity calculations. It seems then that Section 3 would be better served as a description of adjoint modeling, and the background of how this works, rather than or in addition to inverse modeling, as the latter isn't actually done in the present manuscript. This would help clarify, for example, the setup of the adjoint calculations that are performed later for validation in 5.2.1, which I don't believe used a cost function of the type shown here, but rather something different.

Section 3 is necessary to show why the adjoint has been developed and attach consistency to the article. A simplified form of the described cost function is used to validate the adjoint.

5996.15: The forward sensitivity calculation was performed in how many locations? It seems from Fig 3 that they were done in many grid cells, in order to compare to the adjoint results throughout the domain of this figure, but that would be very expensive, computationally, even using Eq 3. If transport was turned off for the testing, all locations could have been tested simultaneously, but this wouldn't constitute a very meaningful test of the adjoint of the tracer transport model.

The forward sensitivity calculation was performed using Eq 3 at the same grid cells as for the adjoint simulation. Indeed it is very expensive, computationally. However, this is very powerful test, as it make possible to compare to the adjoint results throughout the domain.

5.2.1: What was the state vector used for these tests? CO2 initial conditions? Fluxes? Or flux scaling factors? What are the corresponding units of the results shown in Fig 3?

The state vector is flux, the target value is concentration. CO_2 initial conditions and fluxes are same as for the GELCA forward simulations (added to text). The units (ppm/(μmol/m^{2}s)) are added to the figure caption.

5997.10: It would probably be good to show results from these tests somehow.

We revised text as follows: "We use Eq. (7) to test the adjoint model initialized using several different random random vectors **u** and **v**. For all cases, Eq. (7) compares well within machine epsilon with mismatch between -3e^{-14} to 6e^{-14}."

Figs 4-6: These are really interesting results. I found myself, however, having to flip back and forth between these figures to compare across the different modeling approaches. Comparison for a single method across days was much less interesting or relevant to this work. So I would suggest reducing these figures to a single figure that shows the results for a single day but for the 4 methods: eulerian, Lagrangian (native), Lagrangian (aggregated), coupled.

We tried to make the figures easier to compare and combine them appropriately. Section 5.2.2 was revised.

5999: "substantial amount of manual programming effort is required" This should be expanded for a GMD article.

We revised paragraph 5995.1-5 to add more detail about manual code developing, as follows: "The tangent linear and adjoint models of the NIES TM to FLEXPART coupler were derived using the automatic differentiation software TAF (http://www.FastOpt.com), which significantly accelerated the development. However, considerable manual processing of forward and adjoint model codes was necessary to improve the transparency and clarity of the model and to optimize the computational performance of, including MPI, as the TAF code used here (version 1.5) does not fully support MPI routines."

Editorial:

This manuscript needs a thorough proofreading and grammar check prior to publication. I've provided comments below on the abstract and introduction but stopped after that point.

5984.7 tangent –> tangent linear

Revised

5984.6: paragraph break not needed

Revised

5984.11: as results –> as a result

Revised

5984.11: of Eulerian –> of the Eulerian

Revised

5984.17: "test experiments" is redundant, suggest just "tests" or "experiments".

Revised

5984.17: shown –> shows

Revised

abstract: the written tense keeps changing, please try to use a single tense throughout.

The abstract was rewritten.

5984.20: demonstrates the –> is (or was, depending on if you decide to write in the past or present tense throughout) shows to have

5985.18: a density –>the density

Revised

5985.19: measurements –> more measurements

Revised

5985.21: global scale CO2 observation are not existing–> global scale in situ CO2 observations do not exist

Revised

5986.10 CO2 a –> CO2, a

Revised

5986.12: If tracer is a chemically inert –> For chemically inert tracers,

Revised

5986.15: running multiple times with set –> run multiple times with different sets of

Revised

5986.19: Seems odd to have the paragraph break here, instead of e.g. line 22.

Revised

5986.29: “memory demands” should be minimal for adjoint approaches with inert tracer transport (i.e. linear) models.

Indeed, the adjoint approach has relatively low CPU and memory demands. However, here we pointed out computational cost of Eulerian chemical transport models (CTMs) with the high-resolution grids in adjoint and forward simulations.

5987.1 “It would. . ..fluxes” This sentence doesn’t make much sense, and needs to be rewritten.

Revised as follows: “It would be beneficial to increase the model resolution close to observation points, where the strong observation constraint can significantly improve the optimization of the resulting emission fluxes.”

5987.10: utilize of the –> utilize the

Revised

5987.11: the adjoint, which –> an adjoint that

Revised

5987.17: “One goal” is there another goal of this work? Forward model evaluation perhaps? If so this other goal should also be directly stated. If not, suggest saying “The goal”.

Revised. “The goal of this study is …”

Eq 1: why does the “l” index start at 0 and the others at 1?

“l” is a time index, while others are coordinates