Supplement of

Improved ELMv1-ECA simulations of zero-curtain periods and cold-season CH$_4$ and CO$_2$ emissions at Alaskan Arctic tundra sites

Jing Tao et al.

Correspondence to: Jing Tao (jingtao@lbl.gov)

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Table S1 – Location, vegetation and mean annual temperature of ABoVE sites\textsuperscript{1}.

| Site Name | Full Name                               | Site Location | Vegetation                                                                 | Observed Mean Annual Air Temperature (°C) |
|-----------|-----------------------------------------|---------------|-----------------------------------------------------------------------------|------------------------------------------|
| BEO       | Barrow Environmental Observatory        | 71.2810, 203.3877 | Moist acidic tundra - wet sedges, grasses, moss, and assorted lichens.     | -11.3                                    |
| BES/CMDL  | Biocomplexity Experiment, South;         | 71.2809, 203.4035 | Moist acidic tundra - wet sedges, grasses, moss, and assorted lichens       | -11.3                                    |
| ATQ       | Atqasuk                                 | 70.4696, 202.5911 | Moist-wet coastal sedge tundra and moist-tussock tundra                    | -10.8                                    |
| IVO       | Ivotuk                                  | 68.4865, 204.2498 | Polar tundra                                                               | -8.9                                     |

\textsuperscript{1} https://daac.ornl.gov/ABOVE/guides/AK_North_Slope_NEE_CH4_Flux.html
Table S2 – List of tested moisture- and temperature-functions. The environmental modifier is $f(W) \times f(T) \times f(O) \times f(D)$ or $f(W) \times f(T) \times f(D)$ when using moisture scalars that already incorporate oxygen stress, including Standcarb (Harmon and Domingo, 2001), Daycent (Kelly et al., 2000), Skopp (Skopp et al., 1990), Moyano (Moyano et al., 2013), and Yanetal (Yan et al., 2018). Details about the scalars are provided in Sierra et al. (2015) and Yan et al. (2018). Combining the 22 moisture scalars and 37 temperature scalars resulted in 814 environmental modifiers to the base decomposition rate.

| No. | W Scalar* | No. | T Scalar |
|-----|-----------|-----|----------|
| 1   | Standcarb | 1   | Century1 |
| 2   | Daycent   | 2   | Century2 |
| 3   | Skopp     | 3   | Daycent1 |
| 4   | Moyano    | 4   | Daycent2 |
| 5   | Century   | 5   | LloydTaylor |
| 6   | Demeter   | 6   | Kirschbaum |
| 7   | Candy     | 7   | Demeter |
| 8   | Gompertz  | 8   | Standcarb |
| 9   | Myers1    | 9   | $Q_{10} = 1.3(T_{ref}=10)$ |
| 10  | Myers2    | 10  | $Q_{10} = 1.4(T_{ref}=10)$ |
| 11  | ELM-S0 (minpsi = -10 Mpa; ELM Default) | 11  | $Q_{10} = 1.5(T_{ref}=10)$ |
| 12  | ELM-S1 (minpsi = -1000 MPa) | 12  | $Q_{10} = 1.6(T_{ref}=10)$ |
| 13  | ELM-S2 (minpsi = -10^6 MPa) | 13  | $Q_{10} = 1.7(T_{ref}=10)$ |
| 14  | Yanetal (Sf_op=0.50; b=0.50) | 14  | $Q_{10} = 1.8(T_{ref}=10)$ |
| 15  | Yanetal (Sf_op=0.65; b=0.50) | 15  | $Q_{10} = 1.9(T_{ref}=10)$ |
| 16  | Yanetal (Sf_op=0.80; b=0.50) | 16  | $Q_{10} = 2.0(T_{ref}=10)$ |
| 17  | Yanetal (Sf_op=0.50; b=0.75) | 17  | $Q_{10} = 2.1(T_{ref}=10)$ |
| 18  | Yanetal (Sf_op=0.65; b=0.75) | 18  | $Q_{10} = 2.2(T_{ref}=10)$ |
| 19  | Yanetal (Sf_op=0.80; b=0.75) | 19  | $Q_{10} = 2.3(T_{ref}=10)$ |
| 20  | Yanetal (Sf_op=0.50; b=1.0) | 20  | $Q_{10} = 2.4(T_{ref}=10)$ |
| 21  | Yanetal (Sf_op=0.65; b=1.0) | 21  | $Q_{10} = 2.5(T_{ref}=10)$ |
| 22  | Yanetal (Sf_op=0.80; b=1.0) | 22  | $Q_{10} = 1.3(T_{ref}=25)$ |
| 23  |         | 23  | $Q_{10} = 1.4(T_{ref}=25)$ |
| 24  |         | 24  | $Q_{10} = 1.5(T_{ref}=25)$ (ELM Default) |
| 25  |         | 25  | $Q_{10} = 1.6(T_{ref}=25)$ |
| 26  |         | 26  | $Q_{10} = 1.7(T_{ref}=25)$ |

* Oxygen stress already built in Standcarb, Daycent, Skopp, Moyano, and Yan et al. functions.
Table S3: Parameters related to methane processes and the default and tested values. We conducted seven parameterizations for sensitivity tests on the methane process.

| Variables | Long name | Default Value (Reference values in Riley et al. (2011)) | Tested New Value | Parameterization |
|-----------|-----------|---------------------------------------------------------|------------------|------------------|
| \( f_{CH_4} \) | Fraction of anaerobically mineralized C atoms becoming CH4 | 0.2 (0.2) | 0.5 | New Def.\# Def. New Def. New New |
| \( R_{o,max} \) | Maximum oxidation rate constant for saturated conditions | 1.25E-05 ([1.25E-06, 1.25E-04]) | 1.25E-06 | Def. New Def. New New Def. New |
| \( \varepsilon_{aere} \) | A factor representing remnants of aerenchyma tissues during cold seasons and possible pathways via ice cracks | 0.01 | 0.05 | Def. Def. New Def. New New New |

* Newly introduced into the methane model.
# Def. means the default value.
Table S4: RMSE (°C) of simulated soil temperatures with the original phase-change (PC) scheme and newly resized PC scheme. NaN represents the cases when observations are not available.

| Model Layer (Node Depth) | BES&CMDL | BEO | ATQ | IVO |
|--------------------------|----------|-----|-----|-----|
|                          | Ori_PC   | New_PC | Ori_PC | New_PC | Ori_PC | New_PC | Ori_PC | New_PC |
| Layer 1 (0.01 m)         | 5.66     | 3.82 | 5.45 | 3.85 | 6.47 | 3.77 | 9.12 | 5.42 |
| Layer 2 (0.03 m)         | 5.36     | 3.35 | 5.16 | 3.45 | 6.42 | 3.66 | 9.08 | 5.22 |
| Layer 3 (0.06 m)         | 5.32     | 3.16 | 5.16 | 3.28 | 6.38 | 3.54 | 8.87 | 4.91 |
| Layer 4 (0.12 m)         | 5.25     | 2.92 | 5.22 | 3.00 | 6.33 | 3.40 | 8.87 | 4.81 |
| Layer 5 (0.21 m)         | 5.15     | 2.72 | 4.90 | 2.82 | 6.24 | 3.32 | 8.76 | 4.60 |
| Layer 6 (0.37 m)         | 4.70     | 2.56 | 4.70 | 2.56 | 6.15 | 3.50 | 8.67 | 4.42 |
| Layer 7 (0.62 m)         | 4.41     | 2.33 | 4.41 | 2.34 | NaN | NaN | 8.38 | 4.08 |
| Layer 8 (1.04 m)         | 4.23     | 2.13 | 4.22 | 2.14 | NaN | NaN | 7.75 | 3.46 |
| Layer 9 (1.73 m)         | 4.33     | 2.04 | 4.32 | 2.07 | NaN | NaN | NaN | NaN |
| Layer 10 (2.86 m)        | 4.28     | 2.19 | 4.27 | 2.22 | NaN | NaN | NaN | NaN |
| Layer 11 (4.74 m)        | 3.96     | 2.11 | 3.96 | 2.13 | NaN | NaN | NaN | NaN |
| Layer 12 (7.83 m)        | 2.92     | 1.51 | 2.92 | 1.52 | NaN | NaN | NaN | NaN |
| Layer 13 (12.93 m)       | 2.77     | 0.74 | 2.78 | 0.78 | NaN | NaN | NaN | NaN |
| Layer 14 (21.33 m)       | NaN      | NaN | NaN | NaN | NaN | NaN | NaN | NaN |
| Layer 15 (35.18 m)       | NaN      | NaN | NaN | NaN | NaN | NaN | NaN | NaN |
Table S5 – RMSE (-) of simulated soil liquid water content \(S_{f_{liq}} = \theta_{liq}/\theta_{sat}\) with the original phase-change (PC) scheme and newly resized PC scheme.

|      | BES&CMDL | BEO | ATQ | IVO |
|------|----------|-----|-----|-----|
|      | Ori_PC   | New_PC | Ori_PC   | New_PC | Ori_PC   | New_PC | Ori_PC   | New_PC |
| Layer 1 | NaN      | NaN  | NaN  | NaN  | NaN      | NaN  | NaN      | NaN   |
| Layer 2 | NaN      | NaN  | NaN  | NaN  | NaN      | NaN  | NaN      | NaN   |
| Layer 3 | NaN      | NaN  | NaN  | NaN  | 0.27     | 0.26 | NaN      | NaN   |
| Layer 4 | 0.24     | 0.24 | NaN  | NaN  | 0.23     | 0.15 | 0.31     | 0.27  |
| Layer 5 | 0.21     | 0.17 | NaN  | NaN  | 0.27     | 0.16 | 0.18     | 0.18  |
| Layer 6 | NaN      | NaN  | NaN  | NaN  | 0.37     | 0.28 | 0.24     | 0.20  |
| Layer 7 | NaN      | NaN  | NaN  | NaN  | NaN      | NaN  | NaN      | NaN   |
| Layer 8 | NaN      | NaN  | NaN  | NaN  | NaN      | NaN  | NaN      | NaN   |
| Layer 9 | NaN      | NaN  | NaN  | NaN  | NaN      | NaN  | NaN      | NaN   |
| Layer 10 | NaN     | NaN  | NaN  | NaN  | NaN      | NaN  | NaN      | NaN   |
Table S6 – Moisture-scalar, temperature-scalar, and the methane parameters used for the optimized simulations for each site and the identified generic scheme that provides the best overall performance for all the sites. The tested (1934) “NewPC_NewDecomNewCH4” experiments result in 121 common parameterizations that show satisfactory good performance both in CO2 and CH4 fluxes for all the sites. Among these common schemes, we identified a generic scheme as the one providing the minimum Euclidean distance, calculated as $\sqrt{\sum_{i=1}^{n} dist_i^2}$ where n is number of sites and $dist_i$ is the distance between (NSE_CO2, NSE_CH4) and (1,1) for each simulation. This Euclidean distance evaluates the overall performance for all the sites. The identified generic scheme is identical to the optimized parameterization for BES/CMDL.

| Site         | W Scalar | T Scalar       | CH4 Parameters         | NSE_CO2 | NSE_CH4 |
|--------------|----------|----------------|------------------------|---------|---------|
| BES/CMDL     | ELM-S1 (minpsi = -10^3 MPa) | Q10=2.0 (Tref=35) | $\varepsilon_{aere}$=0.05 and Ro,max =1.25E-06 | 0.80    | 0.75    |
| BES          | Yanetal (Sf_op=0.65; b=1.0) | Q10=2.5 (Tref=25) | $\varepsilon_{aere}$=0.05 | 0.83    | 0.86    |
| ATQ          | ELM-S2 (minpsi = -10^6 MPa) | Daycent2        | $\varepsilon_{aere}$=0.05 | 0.67    | 0.78    |
The moisture and temperature functions tested in this study are shown in (a) and (b), respectively. ELM’s original moisture scalar predicts zero respiration in subfreezing soils (e.g., ELM layer 5, black; a) when soil liquid water content becomes small under frozen conditions. With revised minimum water potentials (magenta and cyan), ELM’s \( f(w) \) would not drop to zero unless soil temperature becomes cold enough to have a very small supercooled liquid water content and a soil water potential less than the prescribed \( \psi_{\text{min}} \), which effectively prevents zero respiration within top ~50 cm soils during the cold season. Other functions have been tested and documented in Yan et al. (2018) and Sierra et al. (2015).
Figure S2 – Daily soil temperature from observations and simulations at IVO. a) Both simulations use the original organic matter density, driven by CRUJRA forcing (“ELM_CRUJRA”), or with the top layer prescribed to observed temperature (“ELM_ImposeTopTp”); b) Simulations driven by CRUJRA with the original and the newly revised phase-change scheme (denoted by “OriPC” and “NewPC”), and with original and the newly derived organic matter density (denoted by “OriOrgM” and “NewOrgM”). Summer overestimation with the original organic matter density is largely improved by using the newly derived organic matter density.
Figure S3 – Deriving the organic matter density at IVO assuming the observed maximum volumetric water content is porosity based on Equation 3 in Lawrence and Slater (2008). To preserve the shape of the original profile, the newly constructed profile, $\text{OrgM}_{\text{new}}(z) = \text{OrgM}_{\text{ori}}(z) \times \frac{\sum_{i=1}^{n} \text{EstOrgM}(i)}{\sum_{i=1}^{n} \text{OrgM}(i)}$, where $\text{EstOrgM}(i)$ is the estimated organic matter density at the $i$th layer and $n$ is the total number of soil layers with available volumetric water content.

Figure S4 – Comparison between ELMv1-ECA simulated daily GPP and MODIS GPP product (500m 8-day MYD17A2HGF) at two of our sites.
Figure S5 – Comparison of multi-year (2013 - 2017) averaged daily soil temperatures observed (Ts_Obs, black) and simulated with the default (Ts_OriPC, blue) and improved (Ts_NewPC, red) phase-change schemes at BEO (a) and ATQ (b). Simulated moisture saturation with the original (Sf_OriPC; green) and improved (Sf_NewPC; magenta) schemes are shown on the right-hand axes. The horizontal axes indicate days from July to June, with ticks represent the first day of each month. Hatched areas represent durations of zero-curtain periods observed (ZCP_Obs, gray) and simulated (ZCP_OriPC, blue; ZCP_NewPC, red). No baseline ZCP is shown in the 6th layer for the two sites because the maximum annual temperature is below 0°C.
Figure S6 – Observed and ELM-simulated daily soil temperature and liquid water content with the original and new phase-change scheme at IVO as an example.

Figure S7 – Observed and ELM-simulated daily soil temperature and liquid water content with the original and new phase-change scheme at ATQ as an example.
Figure S8 – Monthly CH$_4$ and CO$_2$ net flux simulated for 1934 ensemble members (gray lines). Black open circles are observed monthly averages with the number of daily observations less than 10 days, which are not used for the computation of NSE. See Table 2 for the configuration for each experiment.
Figure S9 – Sensitivity of ELM simulated (a) SWE, (b) snow depth, (c and d) soil temperatures, (e and f) liquid volumetric soil moisture (VSM), (g) heterotrophic respiration (HR), and (h) CO2 flux at ATQ to precipitation-phase partition methods (PPMs). Suspicious snow depth measurements appear during summertime (black line; b). Red lines indicate the simulations with the ELM default PPM, and grey lines are simulations with different PPMs as tested by Jennings and Molotch (2019). Different PPMs result in large discrepancies in the snowfall portion of total precipitation, leading to considerable differences in simulated SWE (a) and snow depth (b). The sensitivity of soil temperatures to snow depth and SWE is affected by 1) saturation of snow thermal insulation capacity (i.e., the levels of snow thermal insulation will not increase with snow depth if it exceeds an effective snow depth) (Slater et al., 2017); 2) rainfall fraction of total precipitation, which will not only influence snow compaction and accumulation process (thus snow depth) and snow mass (thus SWE), but also severely impacts soil water contents; 3) snow coverage, which impacts surface albedo and absorbed solar radiation, outgoing longwave radiation, and thus net radiation; 4) snow thermal conductivity schemes; and 5) active layer thickness and bottom boundary conditions of soil temperature, which resulted from lumped impacts of snow-or-rain partition over the long-term period (1901 to 2017 here). Also, the maximum supercooled liquid water content in frozen soils (e and f) does not dramatically decline with decreases in soil temperature if it drops to a certain level, and thus the substrate availability to microbial respiration does not accordingly decrease either. In general, snow conditions impact cold-season CO2 emissions and net annual CO2 flux; and the integrated impacts of precipitation-phase partition methods and simulated snow condition on cold-season CO2 emissions are smaller than that on warm-season CO2 flux at this particular site. Further investigation will be discussed in Tao et al. (2021).
Figure S10 - (A similar figure as Fig.3 in Zona et al. (2016)). Daily CH$_4$ emissions vs. soil temperatures at 12 cm at two sites. Similarly, as in Zona et al. (2016), we applied a 30-day averaging window to smooth the daily data to produce clear seasonal progressions. Shaded blue areas indicate zero-curtain periods, i.e., [−0.75 °C, 0.75 °C]. At BES/CMDL and IVO, observed seasonal progressions proceed in opposite directions (e.g., from black to green and then to red), while modeled seasonal progressions follow the same clockwise direction.

Figure S11 – Comparison of observed and simulated CH$_4$ emissions at six high-latitude sites as reported in Riley et al. (2011) and Xu et al. (2016). ELMv1-ECA simulated results with the identified generic parameterization (red) demonstrate improvements in seasonality of CH$_4$ emissions at these sites compared to baseline results (green).
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