BioSTEAMConnectors Manual

Introduction to the Module

BioSTEAMconnectors (available at GitHub) is written in Python 3.7 and automates the execution of DayCent and the extraction of the applicable parameters. It then separates out the variables used in TEA and LCA, processes them into the format required by BioSTEAM, and runs BioSTEAM to simulate the biorefinery of interest (the corn stover biorefinery in this study) MESP and GWP for each year DayCent simulated. The module then creates two *DataFrame* objects (a data structure in pandas, a Python package for data analysis), one for MESP and one for GWP, where cost or emission data of the different sectors (feedstock production, logistics and preprocessing, biorefinery) are broken down into the different categories to show how each category impacts the total MESP or GWP.

Specifically, the main functions that make up the module include <code>DayCent</code>, <code>read_full_out</code>, <code>MESPPrices</code>, <code>percornstover</code>, and <code>calc_emissions</code>. The <code>DayCent</code> function automates the execution of <code>DayCent</code> and <code>list100</code> for the specific schedule file, input files, and an optional extension file provided by the users. Executing <code>DayCent</code> will output the desired <code>.csv</code> files and the <code>.lis</code> files. The <code>.lis</code> files can then be used in <code>read_full_out</code> to extract the data from the <code>DayCent</code> output files, and the <code>MESPPrices</code> and <code>calc_emissions</code> functions run <code>BioSTEAM</code> and summarize <code>BioSTEAM</code> outputs into the <code>MESP</code> and <code>GWP</code> <code>DataFrame</code> objects, <code>respectively</code>. Additionally, many utility functions, including <code>auto_type</code>, <code>pull_variable</code>, <code>N2Oindirectcalc</code>, <code>CO2fluxcalc</code>, <code>convertCH4</code>, <code>daystoyears</code>, <code>cropyield</code>, <code>totalCH4</code>, <code>nonsoilcalc</code>, <code>percornstover</code>, <code>add2</code>, <code>valueratio</code>, <code>calc_emissions_mon</code>, <code>output</code>, and <code>reset</code> are also included in the module for data management and unit conversion.

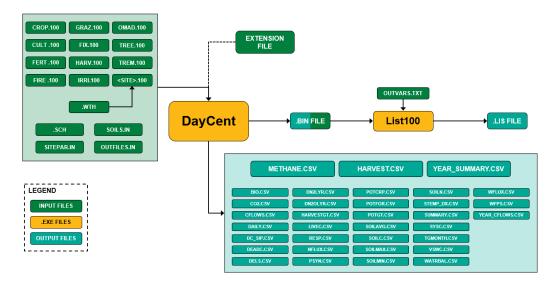


Figure 1. The connection between DayCent and BioSTEAM

Configuration of Workspace

The module workspace must be configured in order to run properly.

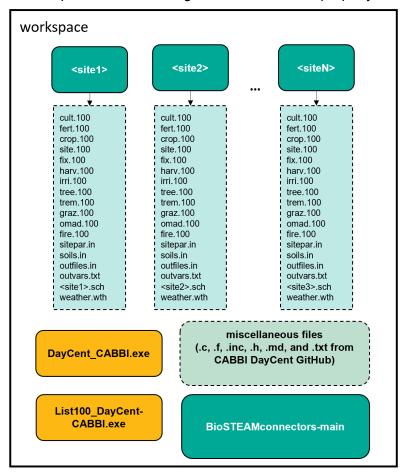


Figure 2. Organization of workspace

The python module uses CABBI's version of DayCent. This can be downloaded from Github at https://github.com/cabbi-bio/DayCent-CABBI by clicking the 'code' button and downloading the ZIP file. Once the GitHub file is downloaded, create a workspace folder. For this example, the workspace folder will be called 'FakeCities' and will be located in my downloads.

Locate the CABBI DayCent code, the name of the ZIP file downloaded is 'DayCent-CABBI-master', and copy over its contents to the workspace folder. After copied over, go into the 'DayCent-CABBI-list100' folder in your workspace, and pull out 'list100_DayCent-CABBI.exe' and place it in the main folder (so instead of the list100 file being in 'FakeCities\DayCent-CABBI-list100\list100_DayCent-CABBI.exe' it will be 'FakeCities\list100 DayCent-CABBI.exe').

The python module must then be downloaded and placed in the workspace. Go to https://github.com/emilypl2/BioSTEAMconnectors and download the code by going to the 'code' button and downloading the ZIP file similar to what was done for the CABBI DayCent. Once the file is downloaded, unzip the folder and place it in the workspace.

Configure your site data into the DayCent acceptable input. Ensure to check the outvars.txt and outfiles.in include all of the files you would like Daycent to generate. While BioSTEAMConnectors supports all of DayCent's outputs, specific files do need to be turned on for the analysis of minimum ethanol selling price (MESP) and global warming potential (GWP) to run. In outfiles.in, year_summary.csv, harvest.csv, and methane.csv must be set to '1'. In outvars.txt, somtc, strmac(2), and volpac must be listed as outputs. List or set these outputs to '1' so that the analysis can run.

Create a folder for each site. The names of the example sites will be 'Hogwarts', 'Metropolis', and 'GothamCity'. In each of these site folders, put in the relevant .100, .in, .txt, .sch, and .wth files as seen in Figure 2. Some of the .100 files are not necessary, so you do not have to have exactly the same files as Figure 2 shows all possible .100 files.

Check that you have all of the files necessary in your site folders and that DayCent and list100 are visible in your workspace. The miscellaneous files will also be visible in the workspace, these run DayCent and do not need any manipulation for the purposes of the BioSTEAMConnectors module.

Running BioSTEAMConnectors

Enter the BioSTEAMConnectors module and press run. The model will ask for the path to your workspace first. For the example, the path is 'Downloads\FakeCities'. This path can be found in your computer's folders.

It will then ask if you are extending a file, DayCent is able to save the state of a model in a binary file which can later be used to initialize subsequent DayCent runs, allowing DayCent to be run in stages; this is called "extending" from the existing binary file. For the example, no we do not want to run an extension so the answer is 'n'.

BioSTEAMConnectors will then ask for your first site folder name. This is 'Hogwarts' for the working example. It will then ask if you would like to add another site. You may be running any number of sites and may continue adding folders until all the sites have been added. Type 'y' if you have another site folder that has not been added yet or 'n' if they have all been added.

For the example, we would write, 'Hogwarts', 'y', 'Metropolis', 'y', 'GothamCity', 'n' to add all 3 folders.

BioSTEAMConnectors will then run DayCent and complete the analysis.

BioSTEAMConnector Outputs

In each site folder, BioSTEAMConnectors will output four analysis excel files in addition to the DayCent generated files. These files are:

Table 1. Output files and descriptions

Name	Description
Allocation Emissions	Global warming potential breakdown for feedstock when using monetary allocation. Breakdowns include total GWP, GWP due to N ₂ O, GWP due to CO ₂ , GWP due to CH ₄ , and GWP due to non-soil emissions. [kg CO2eq/gal ethanol]
Feedstock Emissions	Global warming potential and emissions before allocation. GWP total, and breakdown GWP [kg CO2eq/gal ethanol] between N ₂ O CO ₂ , CH ₄ , and non-soil. Emissions [kg CO2eq/kg feedstock] broken into N ₂ Oflux, N ₂ Oindirect, CO ₂ flux, CH ₄ ox, CH ₄ , and non-soil.
GWPCornstover	Total global warming potential for cornstover including GWP for feedstock (monetary allocation), processing, material, and power.
MESPdf	Minimum ethanol selling price [\$/gal], then broken down to MESP per feedstock emissions, logistic and preprocessing, and biorefinery.