Chapter 15: Earth System Perspective

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Abstract
We review the most current knowledge pertaining to carbon cycle components in an Earth System model and discuss data assimilation applications to inform and improve process-based representations in these models.

Keywords: Earth System model, data assimilation, satellite observations, carbon flux forecasts

1. Introduction and Background: what is an Earth System model?

Earth System models incorporate complex representations of the atmosphere, oceans, land, and ice to diagnose and predict environmental change across different time and space scales. These models have evolved over time from simple, theoretical systems of equations to complex software packages run on some of the world's largest supercomputers. Modern modeling infrastructures focus on a modular structure that supports a unified framework (Figure 1) to be configured many different ways to suit different needs. For example, the model could be configured to simulate atmospheric flow at very high spatial resolution to predict short term changes in weather systems (i.e., days to weeks to months) with simplifications that assume changes in ocean circulation over centennial timescales to be neglected. For century-long climate prediction simulations, a more complex set of processes is required, and the model is run at much coarser resolutions. Despite decades of progress in computing and software engineering, the availability of computational resources still plays a large role in how model experiments are framed, what processes they can include, and what types of output and services they can provide to users.

Atmospheric general circulation models (AGCMs) describe the state of the atmosphere using equations that govern the conservation of mass, momentum, and thermal energy. These equations relate the behavior of temperature, pressure, wind velocity, and moisture and are solved iteratively over a large number of grid boxes covering the Earth. In addition to the fundamental primitive equation that comprise the model's dynamical core, modern general circulation models (GCMs) contain parameterizations that seek to represent processes like thunderstorms, cloud formation, boundary layer turbulence, land-surface hydrology and radiative transfer that are too complex to be explicitly represented at global scales but whose influence must be considered to realistically depict the evolution of weather. These parameterizations also provide information on a much broader set of parameters (for example, soil moisture, surface and top-of-atmosphere radiation, cloud fraction and optical thickness).

Grid box sizes, referred to as the model's resolution, range from single to hundreds of kilometers depending on the application.

When combined with observations for initialization, AGCMs are commonly used to predict the evolution of weather systems 10-14 days in the future. Early numerical weather prediction experiments demonstrated forecasts based on the direct use of observations were unrealistic because small errors in the observed initial state grow quickly over time. Additionally, weather observations are often discontinuous in space and time. Through the mathematical process of data assimilation, observations of the atmospheric state are merged with a modeled background state to create an optimal '*analysis*' that represents the best estimate of current weather. After the analysis is completed, the AGCM is integrated forward in time to produce a forecast. Most weather prediction centers produce new analyses and forecasts multiple times per day, continually ingesting observations from a global network of conventional (e.g., weather balloons, surface stations, aircraft) and satellite observations to revise forecasts. The greatest skill occurs for forecasts in the first few days of the forecast, when the impact of the initialization is greatest. The chaotic nature of the atmosphere means that the precise predictions of events like cold fronts and rainstorms is not possible beyond 2 weeks (Lorenz et al., 1969, Zhang et al., 2019). Weather forecasts are typically produced at as high a spatial resolution as is computationally feasible, currently ~10-km globally, to provide detailed information on severe weather. Traditionally, weather forecasts have been produced using an imposed sea surface temperature boundary condition that does not vary during the forecast period, though this is evolving with some centers now producing forecasts using more complex ocean models (e.g., Morgensen et al., 2018).

Some aspects of the state of the climate can be predicted months in advance when an AGCM is coupled with an ocean GCM (OGCM). While short-term weather forecasts derive skill from a realistic initial picture of the atmosphere, seasonal forecasts estimate the atmospheric response to relatively slow varying changes in boundary conditions (e.g., sea surface temperatures, soil moisture). For example, temperature forecasts over North America draw considerable skill from land surface initialization (Koster et al., 2010). Nearly a dozen organizations worldwide make seasonal predictions of climate using ensembles of coupled atmosphere-ocean GCM (AOGCM) simulations that are generated by perturbing initial conditions and/or model physical parameters (e.g., Kirtman and Min, 2009). The use of ensemble predictions provides a valuable metric for assessing forecast confidence. While numerical weather forecasts have been made since the 1950s, seasonal forecasts have only been made operationally since the 1990s. Though they are considered much less mature, seasonal forecasts are of great interest because of their potential to provide early warnings of a wide array of dangerous and costly hazards. Because of the added complexity and computational cost of simulating both the atmosphere and ocean, seasonal prediction models are typically run at coarser resolutions ranging from 50 to 100 km.

2. Carbon Cycle Modeling in the context of Earth System models

Earth system models (ESMs) combine AOGCMs with modules that describe the evolution of the cryosphere, land biosphere, and atmospheric chemistry to predict changes over decadal and century timescales. They are best known for their use in coupled model intercomparison projects (CMIPs) that support the Intergovernmental Panel on Climate Change (IPCC), the United Nations body responsible for assessing the science of climate change. ESM experiments can be run in several ways. First, they can use as input specified atmospheric concentrations of greenhouse gases whose changes over time have either been estimated by separate models that take into different scenarios of human activity. Second, they can be run with an interactive carbon cycle that influences the concentration of CO_2 over time, adding a higher degree of complexity to simulations. Models with interactive biogeochemistry have only been included in IPCC CMIPs since 2013 (Taylor et al., 2012). The most recent IPCC CMIP incorporates both types of simulations in its standard set of experiments and modeling groups are invited to participate in a wide range of voluntary additional experiments which seek to investigate key processes in greater detail (Eyring et al., 2016). Several of these experiments are directly related to greenhouse gas changes including one that seeks to quantify the response of the carbon cycle to climate change (Jones et al., 2016) and another that examines the impact of land-use and land-cover change (Lawrence et al., 2016). ESMs continue to evolve in the complexity of processes represented, although the wide range of spatial and temporal scales that need to be captured make this an extremely challenging enterprise (Figure 2). Because of the added complexity, length of simulations, and large data volumes generated, ESM simulations are typically run at resolutions of hundreds of kilometers, much coarser than resolutions used for NWP or seasonal prediction.

High-quality information on current and historical regional greenhouse gas budgets plays a critical role in evaluating and improving ESMs. Results from the 2007 CMIP3 showed that large model differences in land carbon uptake results in differences of several hundred ppm of CO_2 by 2100, dramatically altering the rate of warming the planet experienced (Friedlingstein, et al., 2006). Regional land flux differences between models, particularly in the tropics, were particularly large. Despite substantial model development and increases in the complexity of processes represented, results from the 2013 CMIP5 continued to show such large differences between models that it was not possible to predict whether the land would be a source or sink of carbon by 2100 (Friedlingstein et al., 2013). Evaluation of CMIP5 models showed that the difference between model predictions was related to errors in their estimates of present-day CO_2 concentrations, demonstrating the importance of rigorous model evaluation (Hoffman et al., 2014).

Though less mature, carbon cycle modules are being adapted to make predictions of carbon flux on shorter weather to seasonal timescales. The European Centre for Medium-Range Weather Forecasts (ECMWF) computes land-atmosphere within their Integrated Forecast System (IFS), using information from its weather forecast as input to the carbon module. These estimates are combined with near-real-time estimates of fire emissions that are estimated from satellite observations of fire radiative power (Kaiser et al., 2012) and inventory-based estimates of fossil fuel emissions and ocean carbon uptake to produce high-resolution forecasts of atmospheric carbon dioxide (Agusti-Panareda, 2014). Such forecasts are mainly used by the science community, who can use the spatial distributions of trace gases to plan field campaigns (Balashov et al., 2019), to aid in evaluation of satellite retrievals of greenhouse gases (O'Dell et al., 2018), and as boundary conditions to regional models (e.g., Schuh et al., 2010, Gourdji et al. 2012). Major challenges for such forecasts are the bias in the underlying flux model, which can introduce substantial errors in atmospheric concentrations (Agusti-Panareda et al., 2016), and the long latency of fossil fuel and other emission datasets, which are often not available for a year or more (Weir et al., 2021).

Seasonal forecasts of carbon flux represent a relatively new area of research with the potential to support a wider group of users with information 1 to 9 months in advance. Such predictions make use of either the current state of the climate through use of observationally based ocean climate indices or seasonal forecast meteorology fields from the AOGCMs described above. Forecasts of ocean chlorophyll produced by a model of ocean biology and biogeochemistry show skill in predicting anomalous patterns observed by satellites at lead times of 1-3 months (Rousseaux et al., 2020). Changes in tropical land primary production and fire risk that are associated with different phases of ENSO may also be predictable (Betts et al., 2019), gaining skill from the lagged impact of vegetation soil moisture initialization (Lee et al., 2021). Statistical predictions of fire frequency that make use of a combination of a combination of climate information and recent fire activity also demonstrate the potential to predict fire activity and indicate that in certain regions, the strength of the early part of the fire season can be a useful predictor of late season activity (Chen et al., 2019). More research is needed to assess forecast skill in the extratropics, where tropical ocean temperatures have less predictive power. A limiting factor of predictions using seasonal forecast meteorology is the substantial bias inherent in such products, though this can be minimized with bias correction techniques (Arsenault et al., 2018). Seasonal to interannual predictions of human carbon emissions are typically driven by the quality of predictions of economic indicators, such as GDP, which are most reliable over short timescales and in years without significant economic downturns.

Seasonal forecasts of greenhouse gas fluxes have the potential to bridge the gap in latency between observationally constrained estimates, which are typically delayed by several years, and the current time. This could aid in interpretation of observed changes in atmospheric greenhouse gas observations, helping to separate natural variability from human contributions. In addition, output from many flux models is accompanied by valuable information that could be used to inform a variety of stakeholders about diverse topics like fisheries, ecosystem health, and wildfire mitigation. Interannual to decadal scale predictions receive less attention and funding, but also show promise for prediction (e.g., Payne et al., 2017, Lovenduski et al., 2019).

3. Data Assimilation in Earth System models

Data assimilation is "*an analysis technique in which the observed information is accumulated into the background state by taking advantage of consistency constraints with laws of time evolution and physical properties*" (Bouttier and Courtier, 1999). Although this definition is merely a few decades old, its roots can be traced back to the late eighteenth century when both Gauss and Legendre are credited with simultaneously discovering the core principles behind data assimilation (DA). The fundamental principle in data assimilation is to minimize the squared departure between an estimate, and observations and/or background information, very similar to the approach adopted in a least squares framework. Today DA is more generally cast in a probabilistic framework that formalizes the conjunction of the two states of information (e.g., Tarantola, 2005), and the least squares method is derived as a special case of this much more general probabilistic framework.

3.1 Data Assimilation related to numerical weather prediction

The popularity and recognition of DA has primarily stemmed from its application to weather forecasting. Sasaki's trilogy of papers in the Monthly Weather Review (Sasaki, 1970a, b, c) and the subsequent work of Lorenc (1986) and Le Dimet and Talagrand (1986) demonstrated the inherent ability of DA techniques to bring disparate sources of information (i.e., models, various sources of data) to achieve the best analysis, with the analysis being 'better' than the individual pieces of information alone. The current applications of data assimilation have been to merge atmospheric weather observations with a modeled background state to create a realistic, globally continuous field for numerical weather prediction (e.g., Kalnay, 2002). Over time, such techniques have evolved substantially, helping to improve the skill in NWP models. Today, 5-day forecasts are as skillful as 3-day forecasts in the early 1980s (Benjamin et al., 2018), in part because of their ability to ingest approximately more than 5 million observations every 6 hours (Gelaro et al., 2017). Data assimilation methods have also been applied more broadly across the Earth system (Lahoz et al., 2014). Assimilation of ocean observations provide a critical lower boundary condition for seasonal forecasts (e.g., Stockdale et al., 1998, Barnston et al., 1999). As ocean data assimilation has evolved, the datasets assimilated have expanded from in situ temperature and salinity profiles to satellite-based estimates of altimetry, salinity, and sea surface temperature (e.g., Heimbach et al., 2019). The assimilation of ocean color data, which provides information on productivity, is also an active area of research.

3.2 Data Assimilation related to land and ocean carbon cycle

Assimilation of data into land surface models can improve model deficiencies in representing the impact of rainfall on the near surface atmosphere. Additionally, such methods provide important information on root zone soil moisture and carbon flux that cannot be directly observed (e.g., dos Santos et al. 2021). Efforts to directly assimilate vegetation observations such as leaf area index or solar induced fluorescence are increasing with a goal of either optimizing model parameters (Scholze et al., 2007) or constraining flux components like gross primary production (MacBean et al., 2018). However, most current data assimilation systems are unable to take advantage of the increasing array of observations available by assimilating multiple land and vegetation observations simultaneously (MacBean et al., 2016, Smith et al., 2020).

Similar to carbon cycle data assimilation for terrestrial models, assimilation of satellite data may also provide a constraint on properties related to ocean-atmosphere carbon flux over areas not directly observed by *in situ* measurements; however, such capabilities are still being developed. The assimilation of physical state variables such as sea surface temperature and salinity is relatively mature, supporting an array of forecasting and reanalysis efforts. However, most global models used to support near-real time forecasting applications do not include complex representations of ocean biology or assimilate ocean color observations that provide information about productivity. Separate ocean biogeochemical models often rely on observationally derived surface forcing to estimate carbon flux and some include the ability to assimilate ocean color data (e.g., Gregg, 2007). Newer approaches that assimilate both physical state and ocean color data simultaneously are being developed (e.g. Carroll et al., 2020). Such methods are attractive because they have the greatest potential to simultaneously constrain surface conditions, upwelling, and ocean biology, which all influence ocean-atmosphere flux.

3.3 Data Assimilation related to atmospheric carbon observations

Within the last two decades, increasing usage of data assimilation within carbon-cycle research has been in two separate contexts. In an assimilation context, DA has been applied to generate consistent 4-dimensional fields of atmospheric CO_2 concentrations (e.g., Engelen et al., 2009; Chatterjee et al., 2013) or to estimate parameters of biogeochemical models (e.g., Rayner et al., 2005). In this sense, the aim of the carbon DA system is to integrate atmospheric, terrestrial and oceanic data together, along with underlying dynamical constraints into a common analysis framework. Applications that make use of the assimilation framework are built on the premise of carbon cycle model development (e.g., Chatterjee et al., 2013, Koffi et al., 2012, Ziehn et al.,2011) and/or the predictive properties of the carbon system (e.g., Rayner et al.,2011, Ziehn et al., 2011). In addition, DA has gained more popularity in an inversion context (see Chapter 14) for inference of CO_2 sources and sinks using atmospheric CO_2 measurements (e.g., Chevallier et al., 2007, Chatterjee et al., 2012, Basu et al., 2013, Houweling et al., 2015). This application is based on an inverse modeling paradigm, in which the basic premise is that given a set of atmospheric CO_2 observations, and using a model of atmospheric transport, it is possible to infer information on the distribution of CO_2 fluxes at the surface of the Earth (e.g., Enting, 2002). Application to the CO_2 flux estimation problem simply intends to take advantage of the computational efficiency of a DA framework.

It is well-accepted at this point that as carbon science becomes increasingly data rich, DA provides the optimal and most computationally efficient framework to process the high-density data for estimating CO_2 sources and sinks. Simultaneously, rapid advancements are being made in the development of process-based models of the carbon cycle. Atmospheric CO_2 observations provide a valuable constraint on the total carbon budget, but not necessarily on the key signatures of anthropogenic and/or biogenic processes driving those concentration changes. One possible way of inferring information about the processes that influence the surface fluxes of CO_2 may be by examining or incorporating atmospheric measurements of other trace gases in the inversion process. Satellite observations of CO, a species emitted by incomplete combustion from fires, have been used to separate changes in CO_2 related to fires from other types of variability (e.g. J Liu et al., 2017) while observations of NO_2, a short-lived pollutant emitted by fossil fuel combustion, have been used to estimate CO_2 emissions from power plants (e.g. F Liu et al., 2019). The combination of CO, NO_2, and CO_2 data has also been used to identify the emissions fingerprint of different sources (Silva et al., 2017; Figure 3). While assimilation of heterogeneous observation types adds complexity and is currently in early stages, such studies demonstrate the potential for multi-species DA approaches for providing greater information about the processes governing the carbon cycle. Atmospheric assimilation of non-carbon trace gases has also advanced substantially, largely in support of air quality forecasting, helping to pave the way for multi-species approaches to carbon data assimilation.

Applications of such methods are also currently limited because observations of these gases are not made by the same satellite, which can lead to differences in the plume-scale enhancements observed by different satellites (Kuhlmann et al., 2019). Future satellites are being designed with this need in mind. GeoCarb, the world's first geostationary greenhouse gas satellite, is scheduled for launch in 2023 and will measure CO, CO_2, and CH_4 (Moore et al., 2018). ESA's multi-satellite approach, called CO2M and scheduled for launch in 2026, will provide much broader spatial coverage than current sensors and will measure CO_2 and CH_4 along with NO_2. Another challenge in multi-species data assimilation is developing appropriate error correlation statistics, which determine how information from one trace gas influences another.

Most noteworthy is that these data assimilation efforts are fragmented, occurring in different models, using differing data assimilation techniques, over divergent time and space scales. A major challenge over coming years is bringing together these disparate modeling and data assimilation systems. Despite the complexity, such work is a major goal of groups worldwide because of the need for timely, high-quality information about greenhouse gas sources and sinks. Considerable effort is focused on merging land flux and atmospheric greenhouse gas data assimilation with the goal of better understanding the processes controlling land carbon uptake.

4. Future Direction for Carbon Cycle Science, Earth System modeling and DA Applications

An immediate need will be to improve transport modeling capabilities in order to: (a) eliminate systematic biases that may affect inversion results, (b) allow better use of night-time CO_2 measurements or measurements retrieved over complex terrains (e.g. van der Molen and Dolman, 2007, Brooks et al., 2012) from continuous sites, and (c) make better use of satellite data by correctly simulating key processes such as the time scales of stratosphere- troposphere exchange and planetary boundary layer dynamics (e.g., Schuh et al., 2019). Recent efforts have been made in improving certain aspects of the transport model, for example the representation of vertical transport within the planetary boundary layer (e.g., Gerbig et al., 2008) but the community still lacks a pragmatic knowledge of the real magnitude of the transport model uncertainties (Schuh et al., 2019, Crowell et al., 2019). Clearly large- scale efforts (i.e., sustained observations, funding and improved theory) are necessary to improve this critical piece within an atmospheric CO_2 data assimilation framework.

Finally, within the next decade the carbon cycle data assimilation applications will have to transition from an inversion to an assimilation framework. The traditional inversion framework does not support predictive capabilities associated with a true DA framework and lacks the ability to directly adjust the parameters of biogeochemical model components using atmospheric CO_2 observations. In an assimilation framework, however, it is quite feasible to identify which parameters of the biogeochemical model are less well-understood, and subsequently design an observational network/system to constrain those parameters. A research framework adopting an integrated observation and modeling approach may provide the scientific basis for future atmospheric CO_2 mitigation strategies, but it will require a community wide effort to advance current flux estimation systems and link them to prediction systems – the ultimate goal for the majority of Earth System modeling initiatives.

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FIGURES

Figure 1: Bretherton et al. Earth System Model figure (adapted from NASA report, 1988).

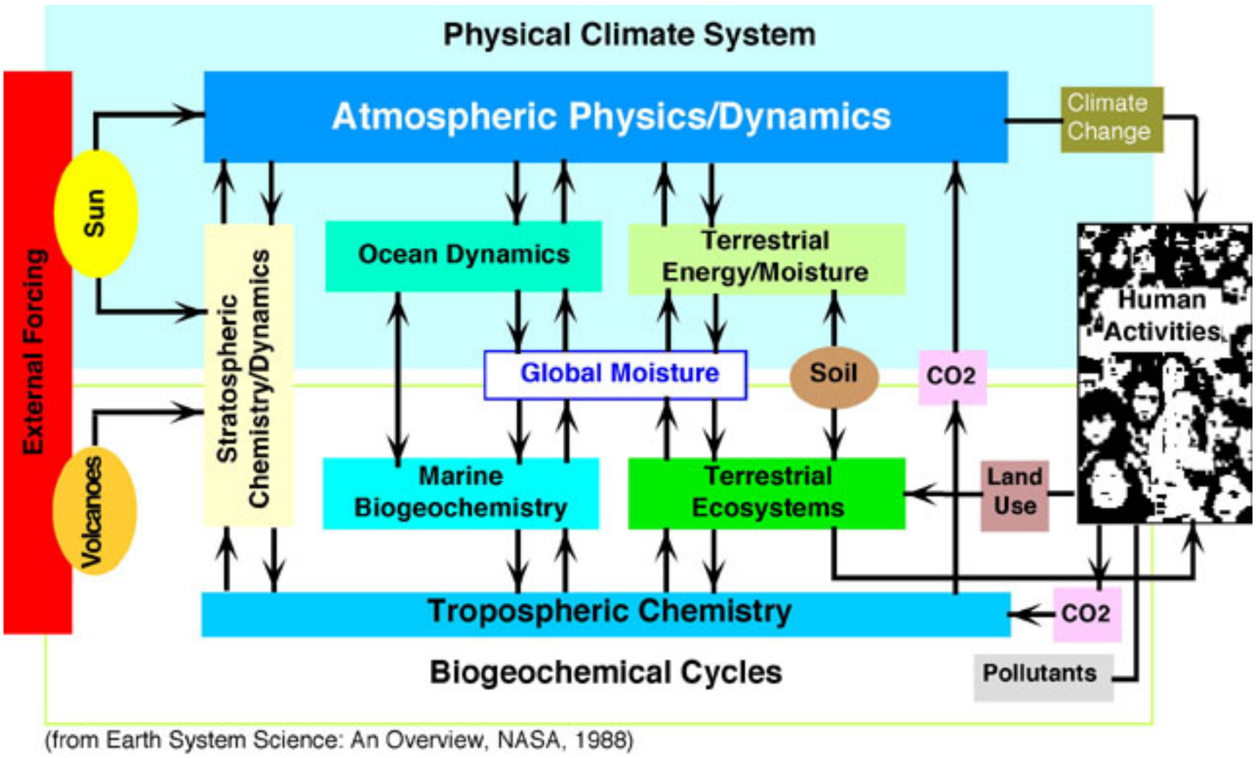

Figure 2a and 2b. Ciais et al. 2014, Figure 1c-1d – example showing range of diverse terrestrial and ocean carbon cycle processes that occur on various space-time scales and need to be incorporated in Earth System models, as well as constrained by observations in a DA context.

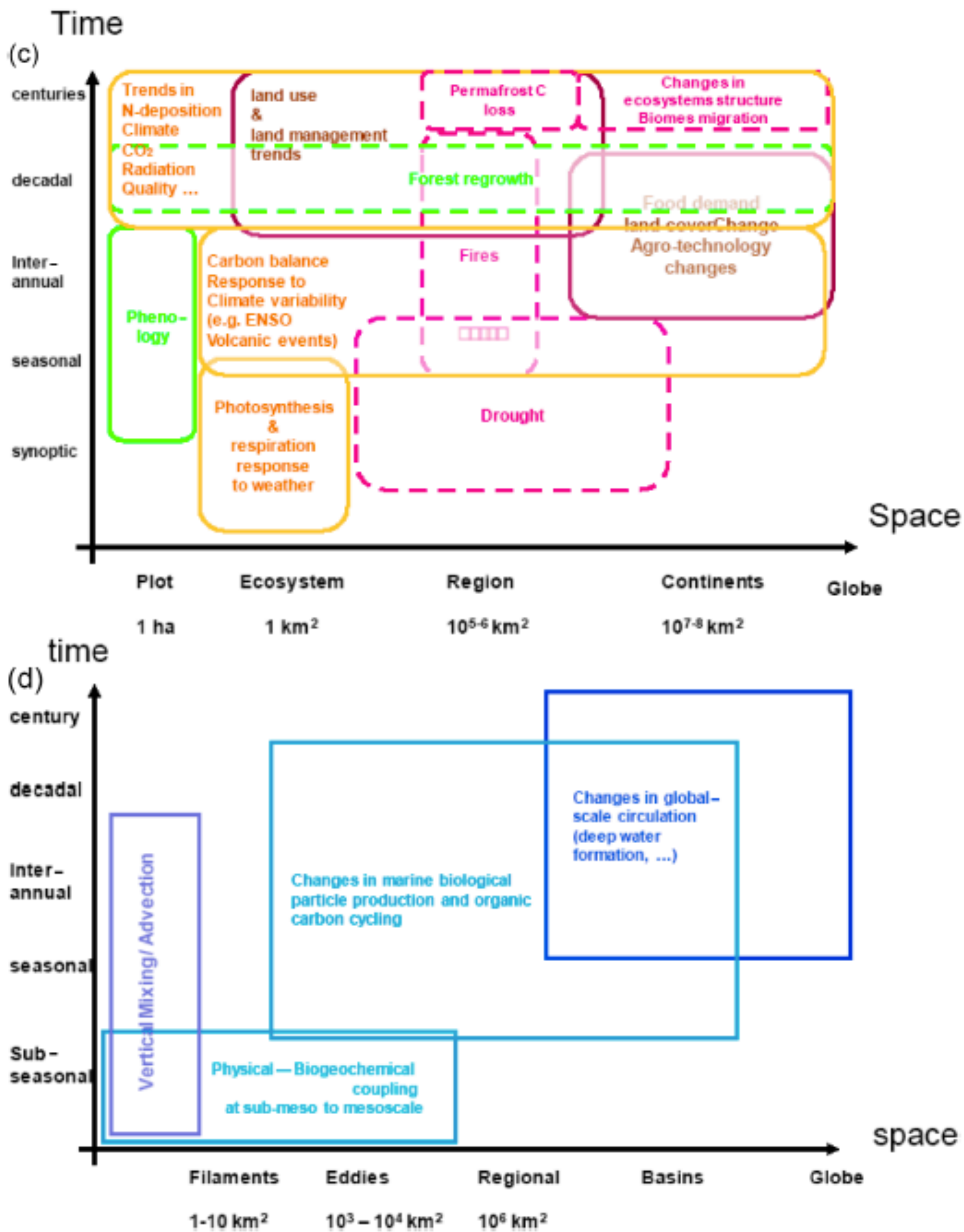

Figure 3 – Across combustion regimes and megacities, distinct relationships between X_{CO}, X_{CO2} and X_{NO2} have been observed (adapted from Silva and Arellano, 2017, Figures 3 and 5). Data

assimilation approaches can be used to analyze joint distribution of various species and reconcile the inconsistencies between observed and modeled emissions.