



Investigating soil health mechanisms through elemental relationships: a systems dynamics approach

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Introduction

Human agriculture is broadly considered as one of human civilization's longest-standing efforts to cultivate predictable outcomes based on systematic, empirical observations (Snir et al. 2015). Ancient farming and animal husbandry techniques grew out of a collective human need to survive local seasonal and climatic shifts in the availability of food and other provisions (Zeder 2011). Agriculture still serves to satisfy those same basic human needs in the modern era. However, the climatic shifts we now need to collectively weather have reached a global scale, and are due to our own use of Earth's resources. In fact, modern intensive agricultural practices not only degrade natural sinks of atmospheric CO₂ through land use changes, but they also lead to greenhouse gas emissions, and overall contribute to human-caused climate change (Tubiello et al. 2022).

A major consequence of agricultural land use practices such as tillage is the significant loss of below-ground carbon content due to soil disturbances (Jackson 2017). As a result, the development of more sustainable agricultural practices has largely focused on modifying growing patterns and frequencies in order to rebuild stocks of soil organic carbon (SOC) in agricultural soils, reduce fertilizer needs, and improve overall soil health, bolstering the resilience of our food system while reducing its greenhouse gas impacts.

At the same time, soil health measurement is a complicated and costly process. For example, the North American Project to Evaluate Soil Health Measurements (NAPESHM) was a project aimed to identify effective indicators of soil health. This project assessed over 20 indicators over 120 long-term research sites from north-central Canada to southern Mexico. In this project, several difficulties were assessed in measurement of soil physical properties, chemical properties, and biological processes. For example, conflicting results often exist when relating soil management processes to soil physical properties such as capture and storage of water (Norris et al. 2020). The measurement of soil chemical properties such as Phosphorus is inherently difficult to standardize due to dependences on soil mineralogy and pH (Norris et al. 2020). Additionally, measuring soil carbon fluxes can be especially difficult due to climate effects varying from years to decades (Norris et al. 2020). Due to these various complications, it is important to understand and measure soil health in a comprehensive way.

One possible way to enhance our understanding of soil health is to build a model framework which can track the relationships and dynamics of different atomic elements in soils in a data-driven way. Elements within soil are understood by farmers to have negative and positive influences on each other, and influence plant growth in predictable ways (Mulders 1965). In this project, I use tools from geology and agronomy to investigate elemental relationships within soil and evaluate whether this information can be used as a tool to both understand and improve soil health outcomes. Soil health can be measured through many indicators and is an important consideration when implementing soil intervention techniques. In this project, a systems dynamics approach was applied towards understanding soil ecosystem relationships — specifically, through the positive and negative influences that different elements in soil had on each other. A holistic visual framework to understand soil elemental relationships was investigated, and in this report I explain my findings.

This project covers three sections: A systems dynamics flowchart, hypergraphs, and Mulder's charts. These three different visual frameworks each portray soil element relationships with a unique style and focus. The flowchart uses a 2-D stock and flow approach to visualize each element, and their positive and negative influences on other elements. Through that flowchart, I identified clear distinctions between elemental influences, with geology and geochemistry driving different correlations. The hypergraphs use an approach similar to a Venn diagram, focusing on the similarities and differences between elements and their shared mineral origins in soil. The Mulder's chart follows an approach common in modern agriculture and combines the two previous versions in a simplified arrow diagram, composed of elements from the hypergraph, with positive and negative influences shown through arrows similar to the systems dynamics diagram.

Systems Dynamics

A systems dynamics diagram is a type of framework that can be used to understand a system of forces that sustain a process or state (Albin 1997). This type of diagram is especially useful in identifying feedback loops, and complex processes and relationships. As a result, this type of diagrammatic approach can help guide the creation of a data-driven framework for analyzing soil elemental relationships. Firstly, the specific variables and influences within a soil system needed to be identified.

This project began by identifying specific elements that can be identified as important within soil growth. These included: Iron, Phosphorus, Zinc, Nitrogen, Potassium, Calcium, and Magnesium. After researching the relationships between the elements, I created a systems dynamics diagram, showcasing their positive and negative influences on each other, and showcasing possible reasons as to why these influences may occur. The diagram, centered around the flux of carbon, portrays the relationship between the separate elements and each other (Figure 1).

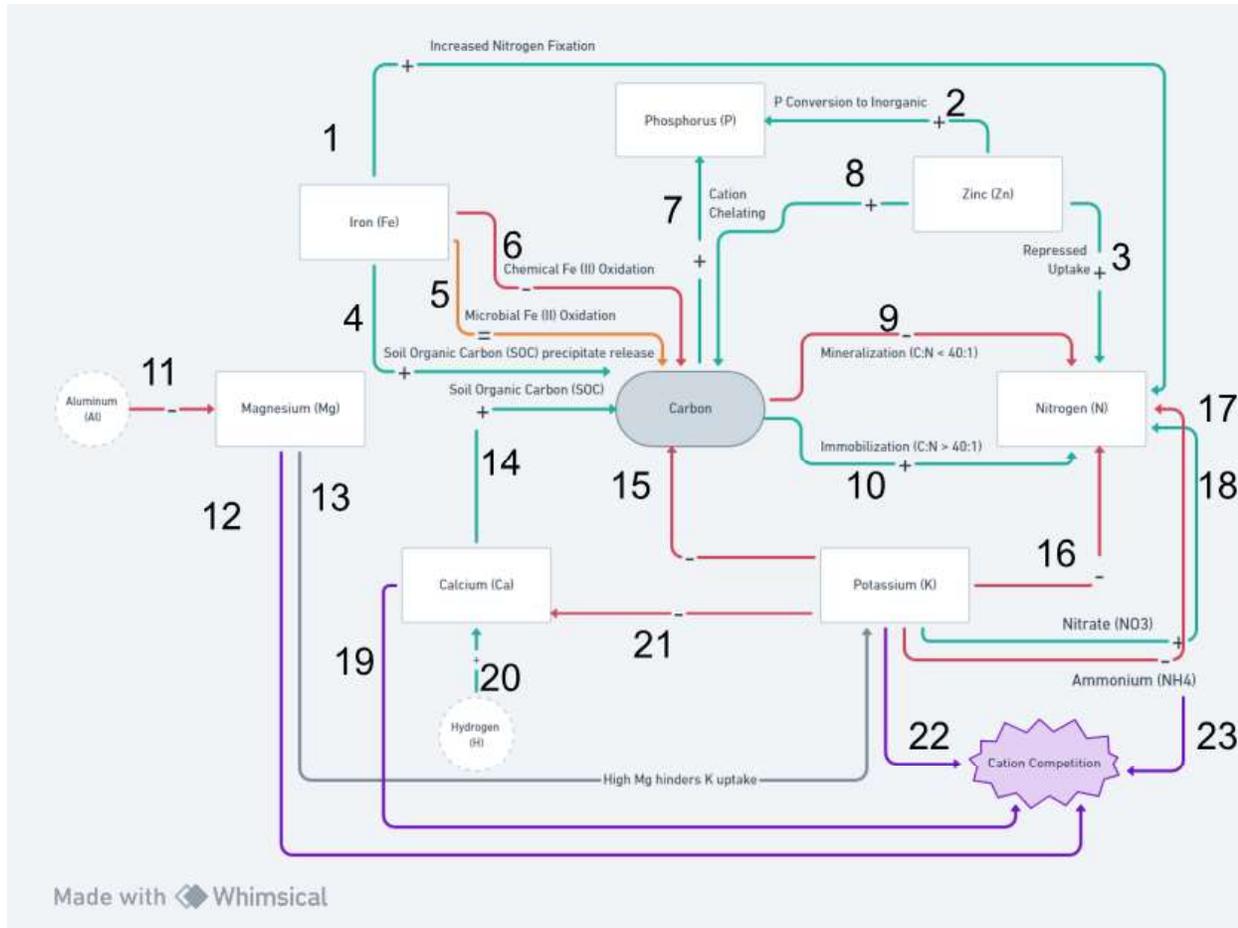


Figure 1. Systems Dynamics Diagram. Soil Elemental relationships.

1. Addition of Fe to soil can increase N-fixing activity (Zhang 2023).
2. High Zn conversion of P from organic to inorganic (Prakash et al. 2018).
3. High Zn repressed uptake of N by plants, improved N availability.
4. Reduction of Fe releases soc from Fe-SOC precipitates (Song et al. 2022).
5. Microbial Fe(II) oxidation stabilizes SOC (Song et al. 2022).
6. Chemical Fe(II) oxidation decomposes SOC (Song et al. 2022).
7. Addition of organic carbon, availability of phosphorus increases due to chelating of polyvalent cations by organic acids and other decay products (Johan et al. 2010).
 - Organic matter is made up of humic substances that have many negative charges and functional groups, such as carboxyl, hydroxyl, and carbonyl. These functional groups react with Al and Fe to form stable complexes, thus preventing their reaction with P (Johan et al. 2010).
8. Positively correlated with soil organic carbon (Thingujam 2019).
9. Mineralization, nitrogen from organic to inorganic (C:N < 40:1), available to plants (Augustin et al. 2010).
10. Immobilization (release N) (C:N > 40:1), from inorganic to organic forms, unavailable to plants (Augustin et al. 2010).
11. Decreased Mg availability with high Al content (Ericsson et al. 1995).
12. Cations compete with each other for a spot on the cation exchange capacity, stronger cations get taken up by plants, which leaves weaker cations to be more present in the soil (McClellan 2023).
13. High soil magnesium may hinder potassium uptake (Richards 2019).
14. There have been studies that show exchangeable Ca positively correlates with SOC (Rowley et al. 2023).
15. Excess Potassium reduces C in roots, as well as being an activator for C metabolic enzymes in plants (Xu 2020).
16. High K generally negative, depending on nitrogen compound (Xu 2020).
17. Potassium has a negative relationship with NH₄ (Xu 2020).
18. Positive with NO₃ (Xu 2020).
19. Cations compete with each other for a spot on the cation exchange capacity, stronger cations get taken up by plants, which leaves weaker cations to be more present in the soil (McClellan 2023).
20. Soil with high Hydrogen can release Ca from soil minerals (Synder 2023).
21. High K can increase uptake of Ca in maize (Xu 2020).
22. Cations compete with each other for a spot on the cation exchange capacity, stronger cations get taken up by plants, which leaves weaker cations to be more present in the soil (McClellan 2023).
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This diagrammatic approach yielded various results. Firstly, biochemical reactions such as mineralization, immobilization, and oxidation, and reduction were highlighted through the influences within nitrogen, iron, and carbon. Immobilization or the release of N occurs when $C:N > 40:1$, while mineralization the absorption of N occurs when $C:N < 40:1$ (Augustin et al. 2010). Oxidation and reduction reactions were present between iron and soil organic carbon. The reduction of Fe can release SOC (Soil organic carbon) from Fe-SOC precipitates, while microbial Fe(II) oxidation can stabilize SOC, and chemical Fe(II) oxidation can decompose SOC (Song et al. 2022). This relationship, similar to mineralization and immobilization, can demonstrate how a single element can both negatively and positively impact another depending on surrounding conditions. Cation competition is another largely influencing factor in the soil system (Saidi 2012). Cations in the soil compete with one another for a spot on the cation exchange capacity. However, some cations are attracted and held more strongly than others. Therefore, when stronger cations like aluminum or calcium are present in the soil, they are more readily taken up by plants than weaker cations like nitrate or potassium.

Other mechanisms are also shown to have influence on elemental relationships, for example, the positive correlation between organic carbon and phosphorus can be due to the availability of phosphorus increasing via the chelating of polyvalent cations by organic acids and other decay products. More context-specific positive and negative influences are also shown, which were observed and tested experimentally through various research projects on specific crops.

However, while creating this system dynamics diagram, one question that I wanted to investigate was which elements were the most important, influential, or common — essentially, which elements were most appropriate to portray. To do so, I decided to look at the relationships between the different mineral sources for elements in soil. This direction presented an immediate challenge, that multiple elements in soil can be connected by the same geological source. It became clear that a more sophisticated way of displaying connections between elements would be necessary to understand such connections visually.

Hypergraphs

One way to display connections between multiple different elements is through hypergraphs. Similar to a Venn diagram, elements and their respective minerals can be connected visually through encompassing circles. These graphs can also be helpful in determining which element is contained in more or less minerals, and therefore portray their geological commonalities.

As a result, hypergraphs of elements and their shared mineral compounds were able to more accurately portray element and mineral relationships than a simple stock and flow diagram. Using the IMA database of mineral properties, we collected chemical formulae for every mineral currently known to science (Lafuente et al. 2015). Then, I plotted them with the HyperNetX Python package (Praggastis et al.). Each dot represents a mineral compound, and each string an element. Figure 2 shows a simple example, where the elements nitrogen, phosphorus, and potassium can be shown along with any known mineral that contains each or any of these elements. Through these connections, the number of minerals containing each element, or any combination of elements, can be visually depicted.

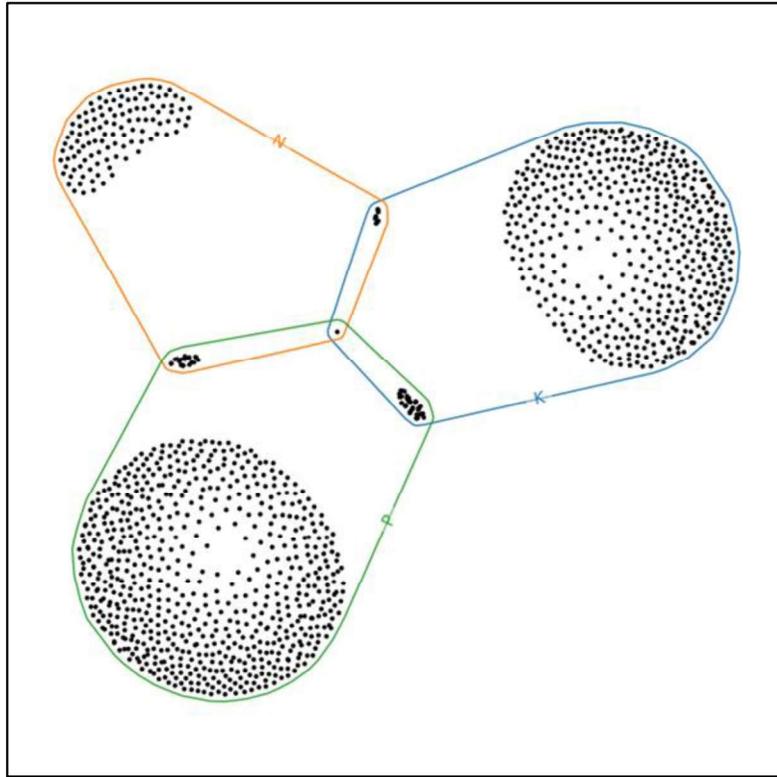


Figure 2. Simple Hypergraph using the elements nitrogen, phosphorus, and potassium.

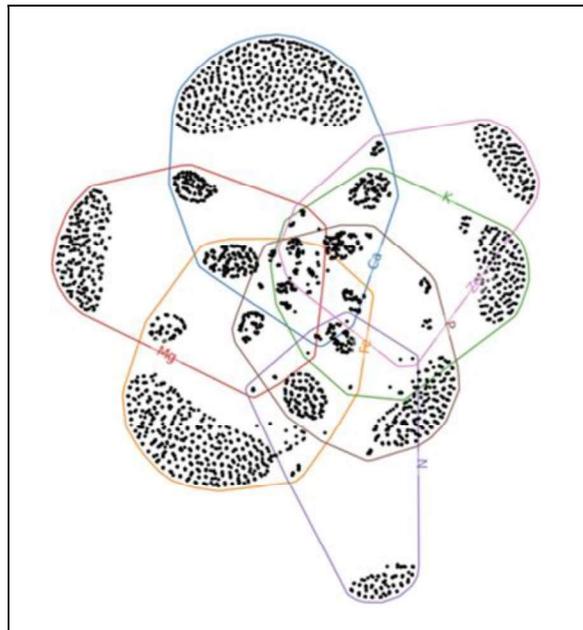


Figure 3. Hypergraph of only the elements in the systems dynamics diagram, Figure 1.

Using hypergraphs, the elements that had the greatest number of mineral compounds in common with each other, can be understood both visually and quantitatively in Figure 4. This step was useful in determining which elements are the most common, and therefore which elements should be represented in the visual framework.

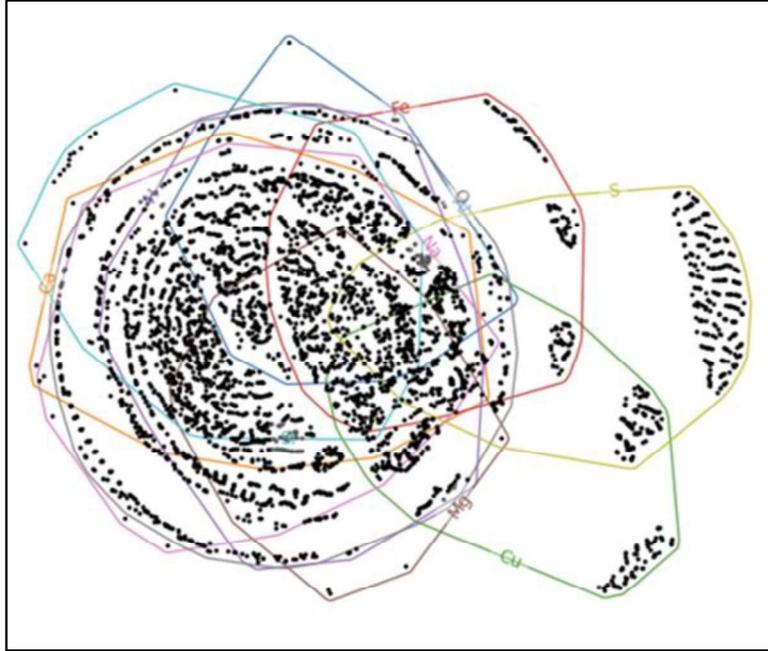


Figure 4. Hypergraph of Top 10 elements with the highest number of minerals.

However, and as shown in Figure 4, the hypergraphs quickly became too complicated to study completely by eye, and the connections they depicted were purely due to mineral data. For the last step of visualization, I wanted to simplify this data and synthesize it with geochemical effects like cation competition in an easy-to-understand way, which can be shown using the Mulder's Chart.

Mulder's Charts

The Mulder's chart is a common chart among the agricultural and farming community, that essentially uses arrows to depict various influences that different nutrients in soil can have on one another. Due to its established reputation among a community that regularly uses soil, this chart would be very useful in creating a new visual depiction of soil elemental relationships. The Mulder's chart not only simplifies the systems dynamics diagram, but also was able to incorporate data from the hypergraphs as the elemental nodes around the chart. Using both my system dynamics research, hypergraph data, and two versions of the Mulder's chart, I created new Mulder's charts, that displayed important elements and their influences towards each other in a simplified way.

In Figure 5, the Mulder's chart was created based off a modern version of the Mulder's chart, containing more elements and more recent data (Fan 2021). In Figure 6, the Mulder's chart was

based off the original version of the Mulder’s chart (Mulder 1953). Both figures utilize the top 10 elements found using the hypergraphs with those that are also present within the elements in the respective Mulder’s chart versions. Interestingly, many of the relationships between the two versions conflict, such as the relationship between calcium and iron changing from mutually negative to positive. However, by creating two different versions, we can portray a more holistic framework that encompasses both old and recent data.

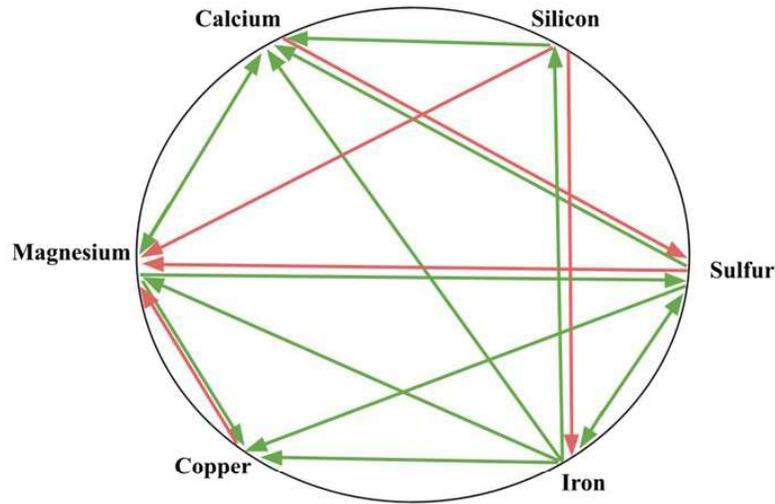


Figure 5. Mulder’s chart based on modern data, using only the top 10 most geologically common soil elements.

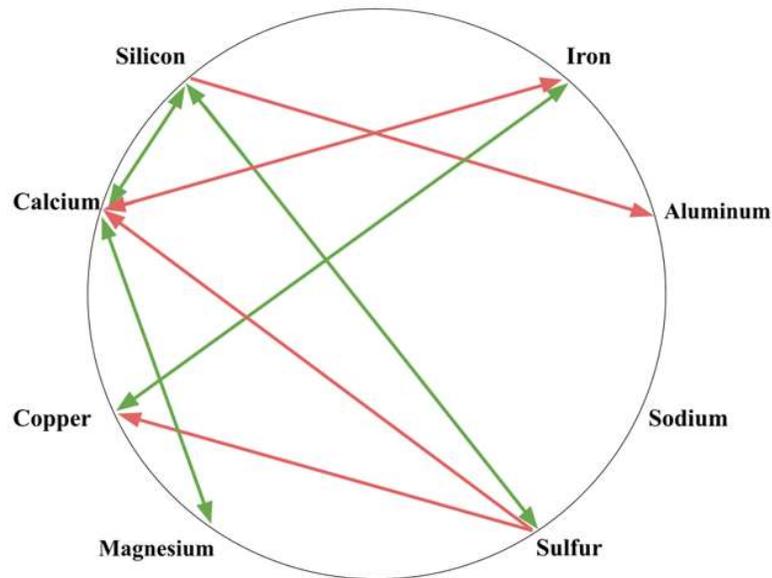


Figure 6. Mulder’s chart based on original data, using only the top 10 most geologically common soil elements.

Discussion

This project led to several insights. Firstly, I reviewed how the presence or absence of different soil elements can be possible indicators of soil health, and confirmed the value in studying elemental relationships within soil more accurately. Then, I worked to diagram the relationships between these soil elements and the sources of their correlations, and I learned that different kinds of interactions should be depicted visually according to the soil scales and subsystems that they connect.

For the next steps of this project, it would be beneficial to build out this framework further, to systematically list out every kind of interaction that can occur between the elemental contents of soil. (It may be sensible to use computational techniques to achieve this step.) Once the framework is in place, the rates of different interactions can be calibrated against real soil measurement data, and the resulting data-driven model could then be used to identify common feedback loops that drive positive sustainability outcomes. It would also be interesting to begin working in soil interactions into environmental, plant, animal, microbial, and water soil interactions, to diversify the influences and relationships accounted for by the model. Lastly, this could be useful in better specifying and achieving goals in soil intervention, such as which nutrients to add to certain soils to increase soil carbon stocks while reducing fertilizer needs, and using the presence or absence of certain nutrients to determine overall soil health.

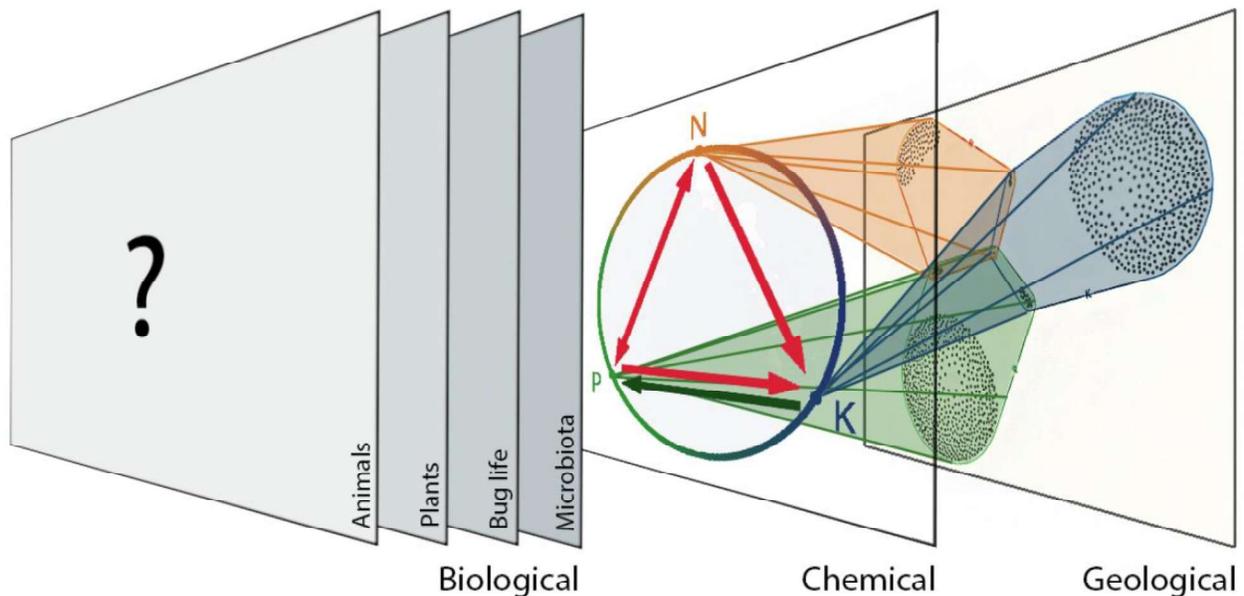


Figure 7: A schematic diagram which breaks down biogeochemical systems into biological, chemical, and geological variables. This initial framework, inspired by systems dynamics, may in its fully developed form be useful in structuring interactions and inferring correlations between atomic populations in soils and biomass. For the simple case of N, P, and K, the hypergraph from Figure 2 demonstrates how geological structures can contribute to positive correlations between atomic abundances. Independently, the Mulder’s Diagram depicts how chemical interactions within a soil environment can lead to increased or decreased relative availability of critical soil nutrients. The connections between the two graphs represent geochemical interactions which induce positive correlations between atomic abundances (e.g. adding more of a potassium-containing mineral increases the pool of K available for soil chemical interactions). Missing from this diagram are atmospheric variables, which can play critical roles in soil nutrient availability (Yu et al., 2015).

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