THE HYDROGEN ECONOMY: A SYSTEM ANALYSIS

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1. Introduction

Analyses by governments, consultants, industry leaders, and nonprofit organizations around the world agree that "clean" hydrogen will play a vital role in the transition to a low-carbon future [12][18][4] [17] [15]. President Biden's climate plan promises that he will "ensure that the market can access green hydrogen at the same cost as conventional hydrogen within a decade" and identifies producing cheap hydrogen from renewable sources as a project for the yet-to-be-established Advanced Research Agency on Climate [18]. Germany's energy transition plan "crucially depends" on carbon-neutral gaseous and liquid fuels such as hydrogen and many other countries are focusing resources into development of their hydrogen economies [17][15].

Hydrogen fuel, when produced with little to no carbon emissions, is particularly attractive because it acts as a buffer to other forms of renewable energy that are variable and dependent on environmental conditions, such as wind and solar. When these renewables are producing more energy than there is demand, the excess energy can be used to make hydrogen fuel, storing it to be used later. Additionally, it can be used in otherwise difficult-to-transition industries, such as long-distance and freight transport and steelmaking [17]. However, most of the 115 million metric tons of hydrogen produced annually today are made using methane steam reforming, which, without carbon capture and storage, is not a low-carbon production option. What's more, in the US, 57% of hydrogen consumed is used for industrial and oil refining, and 38% is used to make ammonia and methanol [15]. Obviously, significant changes must be made to the existing system in order to supply hydrogen fuel at scale and in order to integrate it into existing energy mixes. This fact begins to touch upon the motivation for this study: as the existing hydrogen economy is necessarily scaled up in the coming years and decades, it must also develop sustainably– that is, renewable production facilities, along with efficient, distributed, and well-designed distribution and storage systems, must be designed and constructed.

In this article, we will present and describe our SysML systems engineering model of the reference architecture of the hydrogen economy. Of course, no one knows how the global network of hydrogen production, distribution, storage, and consumption will develop. This model does not in any way attempt to predict this development; instead, we offer an assessment of current system architecture, including novel and test-phase technologies which are generally thought to be realistic and/or probable actors in the near-future hydrogen system. Therefore, the reference architecture we model could be applied at a global or national scale, and could be revised to more accurately represent a specific instantiated scenario or context.

2. Defining the System

The complexity of the hydrogen economy calls for an intricate understanding of the formal and functional architecture. At the outset, it is imperative to define a clear systems boundary that encompasses all the crucial formal elements while abstracting out unnecessary parts by treating them as inputs and outputs of the system.

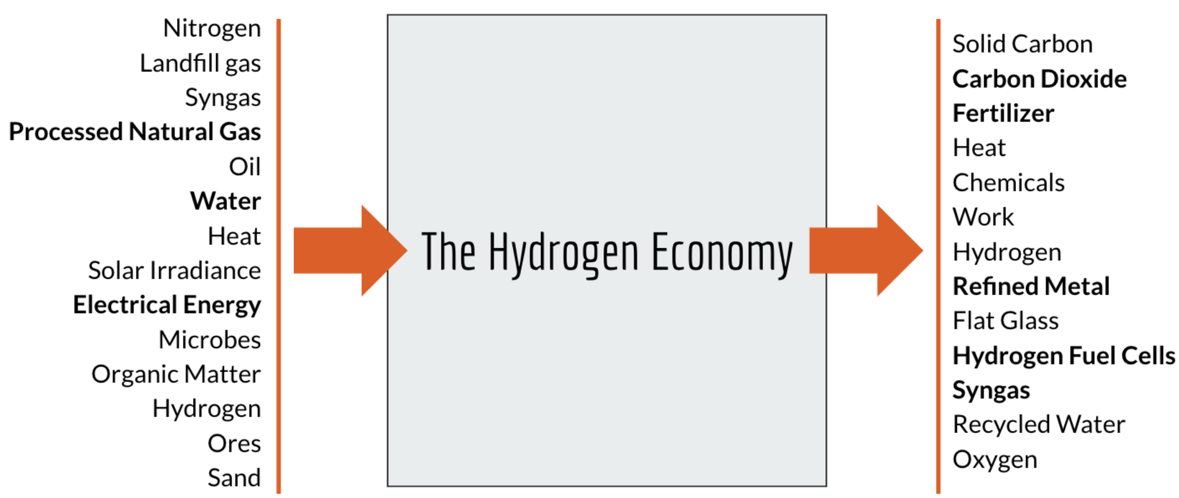

Figure 1 Black Box Diagram of the Hydrogen Economy *The system boundary includes all processes with hydrogen as the operand. The black box diagram abstracts away internal processes and form, showing inflows and outflows of the system, with the most relevant and largest flows bolded.*

For the purposes of this model, the system will include all processes for which hydrogen is the operand. Therefore, major flows into the system will include raw materials used to produce hydrogen, including water, and energy used in the various production processes. Correspondingly, flows out of the system will be pure hydrogen, water, carbon dioxide, and derivatives of hydrogen such as fertilizer and refined metals; consumption of hydrogen is included within the system boundary. Despite the fact that hydrogen use is currently dominated by the oil refining and chemical industries, we have identified potential energy, in the form of fuel, as the primary externally delivered value-related function of the system, along with pure hydrogen to be used as an ingredient in chemical processes.

Hydrogen's most valuable attributes – its versatility and abundance – is manifested in the complexity of the hydrogen economy. Its versatility means that hydrogen may be used in a myriad of applications, and so the hydrogen economy system interfaces with many other systems, such as industrial (for example metals and fuel cell production), energy, electric, infrastructural and built, heating and cooling, chemical, agricultural, transportation, and oil systems [17][4]. The physical interfaces of the hydrogen economy with these systems are mostly at consumption and storage locations (Table 1). The fact that hydrogen can be produced via electrolysis additionally interfaces this system with water systems at production sites.

In consideration of the nature of the system, this paper utilizes block definition diagrams and a design structure matrix. Three levels of the formal architecture are examined and the functional architecture of the hydrogen economy from the production of hydrogen to the consumption of hydrogen is analysed.

The hydrogen economy value chain consists of three primary activities: hydrogen production, hydrogen storage and transportation and hydrogen consumption. This decomposition of the hydrogen economy nicely defines the first level of the formal architecture as shown by Figure 2 as well as the swim lanes of the functional architecture as shown by Figure 3.

Table 1: Interfaces with the Hydrogen Economy

Interfacing System	Physical Interface
Industrial	Steel production facilities Ore refining facilities Glass production facilities Explosives manufacturing facilities Container-filling facilities
Fuel Cell Production	Fuel cell filling facilities Hydrogen vehicles
Energy	Large-scale utility storage locations Steam methane reforming plants Methane distribution pipes Hydrogen derivative production facilities
Electric	Renewable energy production sites Utilities
Infrastructural and Built Environment	Stoves Heating and cooling systems
Chemical	Methanol production facilities
Agricultural	Fertilizer production facilities
Transportation	Hydrogen fueling stations Fuel cells Hydrogen vehicles and freight vehicles Ships
Oil	Petroleum refining facilities
Water	Electrolyzers Offshore windmills Concentrated solar plants All consumption locations of hydrogen fuel (because water is a product of the combustion reaction)

Each formal category is further decomposed into sub-blocks. These elements of form perform one or more activities to produce, transport, store, or consume hydrogen. The Design Structure Matrix (Figure 3) presents the principle elements of form that make up the level 2 architecture of the system. As we can see, the formal structure is relatively linear: the elements of hydrogen production are each connected to some elements of transportation and storage, and these elements in turn are connected to locations of storage and consumption.

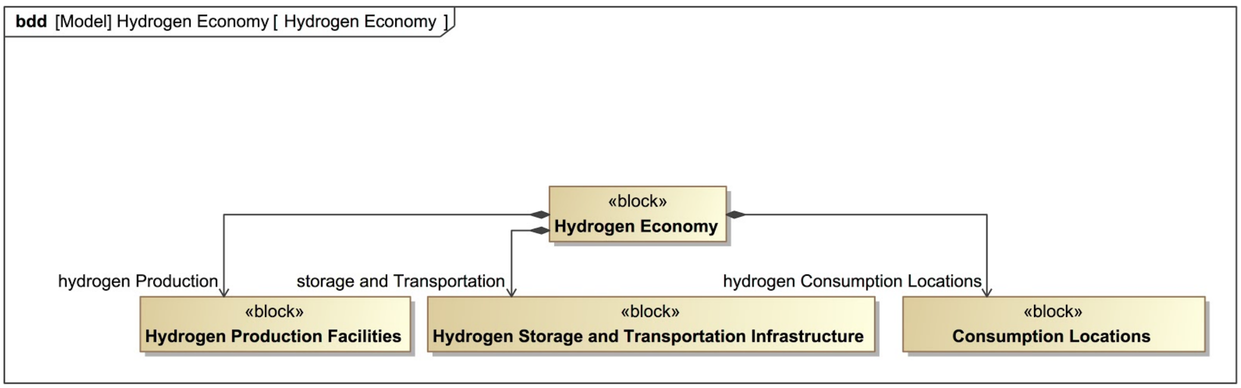

Figure 2 Hydrogen Economy Block Definition Diagram *At the highest architectural level, the hydrogen economy consists of production facilities, storage and transportation infrastructure, and consumption locations.*

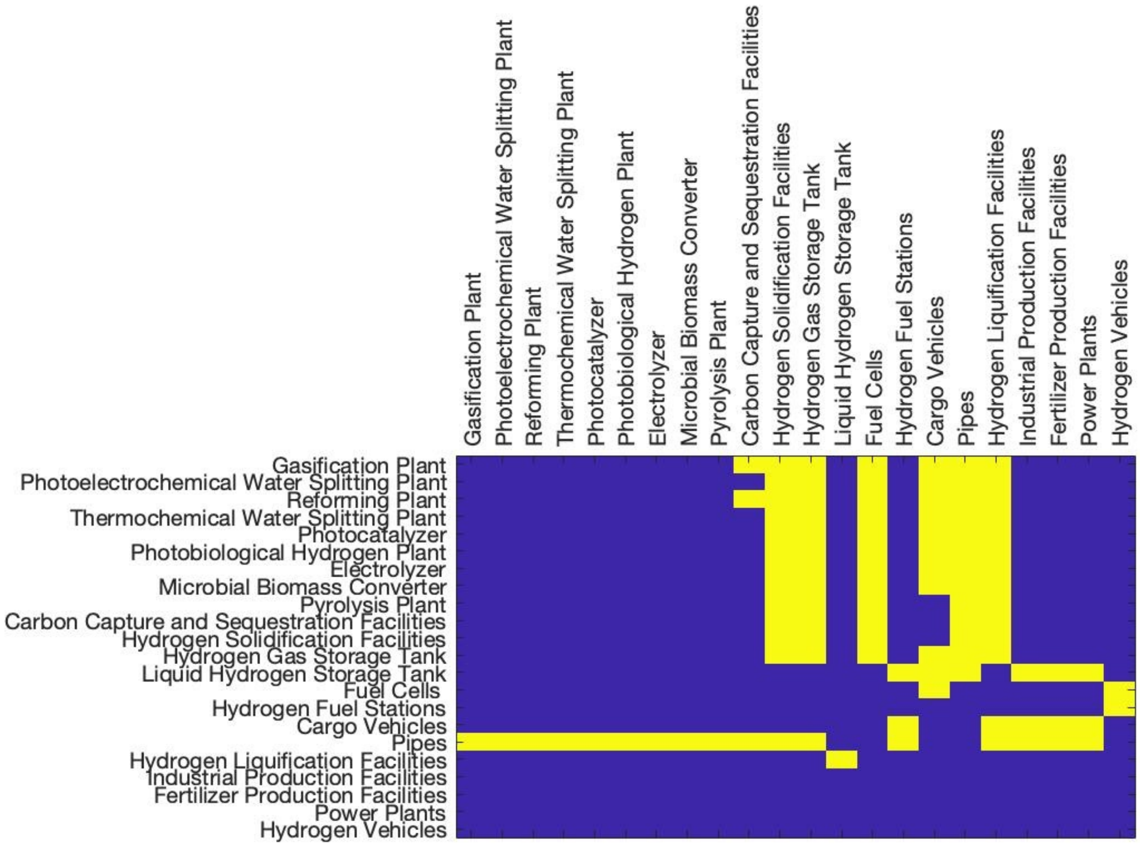

Figure 3 Hydrogen Economy Design Structure Matrix *This matrix shows the formal relationships between elements of the level 2 architecture of the Hydrogen Economy. Yellow squares represent a physical connection from the row title to the column title.*

Of note are the different levels of scale at which the various system elements operate. As can be seen in Figure 3, not every hydrogen production facility type is connected to every type of transportation or storage, and in turn, each transportation or storage element is connected only to specific consumption locations. These connections are mostly determined by the scale at which hydrogen is being produced. For example, steam methane reforming (SMR) benefits significantly from economies of scale, and so these facilities are usually large and produce large quantities of hydrogen; therefore clients who consistently buy very large amounts of hydrogen (such as utilities or refineries) are more likely to buy from these production facilities than smaller, distributed production facilities. This model is ideal for, and could enable the construction of, direct pipelines from the production site to the storage or consumption site. On the other hand, electrolyzers and photocatalyzers don't benefit from the same economies of scale as steam reforming, and so are more likely to be distributed and located at the location of consumption, such as at a fueling station. These smaller amounts of hydrogen are more likely to be packaged for transport by freight trucks or ships, and to be delivered to smaller-scale consumers, such as glass production plants and buildings. To gain a better understanding of the hydrogen economy, this paper examines each of the three primary activities of the hydrogen value chain identified above.

3. Hydrogen Production

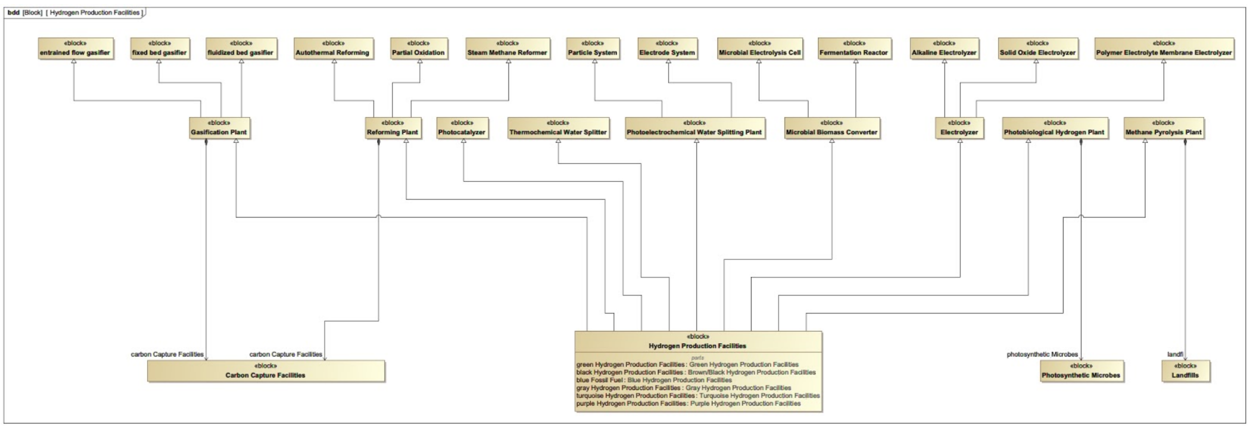

Figure 4 Hydrogen Production Facilities Block Definition Diagram *The class Hydrogen Production Facilities specializes into many different methods of production and their associated forms; currently the most developed and affordable production methods are steam methane reforming and electrolysis.*

As previously mentioned, the current primary method of hydrogen production is steam methane reforming, which produces "gray hydrogen." Water steam is reacted with natural gas to produce pure hydrogen and carbon dioxide; hence, this fossil fuel-based method of hydrogen produces CO2 emissions [16]. Sometimes SMR facilities are equipped with carbon capture and storage technology, and so categorized as producing "blue hydrogen" [17]. Ideally, all future SMR plants should be equipped with CCS, and fortunately existing plants can be retrofitted with CCS, theoretically making them carbon neutral. However, in practice, there are many upstream emissions associated with methane, and carbon capture rates for steam methane reforming are generally 55-90% [17]. Therefore, in order to transition to a truly low-carbon system, other methods of hydrogen production should be prioritized, and SMR may act as a transition production method as the hydrogen economy grows [17]. This is also true of other hydrogen production methods based on fossil fuels, such as methane pyrolysis, which produces "turquoise hydrogen" and solid carbon, and coal gasification [4].

One of these other methods is electrolysis, in which hydrogen is produced directly by splitting water into its constituent elements. The only products of the electrolysis reaction are hydrogen and oxygen, and the inputs are water and energy. The reaction occurs in an electrolyzer, which is composed of an anode, cathode, and electrolyte. Electrolyzers are categorized by their electrolyte, of which there are three main types. In polymer membrane (with a solid polymer electrolyte) and alkaline (traditionally with liquid alkaline solution electrolytes, although solid ones are in the R&D stage) electrolyzers, water at the anode reacts to produce hydrogen ions, which move across the membrane to the cathode as the free electrons flow through an externally driven circuit to the cathode, where the hydrogen ions react to form pure hydrogen gas. Solid oxide (with solid ceramic electrolytes) electrolyzers operate at much higher temperatures (700-800˚C), but are not as electricity-intensive as the other two [6].

If the electrical energy used to split water molecules comes from renewable and carbon-free sources, then the reaction produces "green hydrogen," making electrolysis nearly perfect from a carbon emissions perspective. Additionally, electrolyzers don't benefit from the same economies of scale as SMR, and so can range from appliance-sized for small-scale distributed production to utility-sized (electrolysis source). The challenge with electrolysis is its huge electricity requirement: estimates show that electricity accounts for over half of the cost of electrolysis if the electrolyzer operates around 5,000 full-load hours [17]. As such, decreasing renewable energy production costs will help make electrolysis plants a more viable and attractive alternative to SMR.

There are a number of other green hydrogen production methods, though most require more research and development to become economically viable [10]. Thermochemical water splitters use high temperatures produced by excess nuclear heat or concentrated solar towers to drive a series of reactions, taking in water and recycling its chemical reactants each cycle [10]. In photoelectrochemical methods, a special class of semiconductors are exposed to sunlight to split water directly to produce hydrogen [9]. Finally, biologically-driven hydrogen production, via fermentation (microbial biomass conversion) or direct water splitting (photobiological production) could be a low- to no-carbon method for hydrogen production in the future [7][8]. The infrastructure needed for these processes, and their current and predicted production efficiencies, suggest these production methods will operate at larger, centralized scales [7][8][9][10]. Continuous research and developments are seen in the field of hydrogen production (Guanyu).

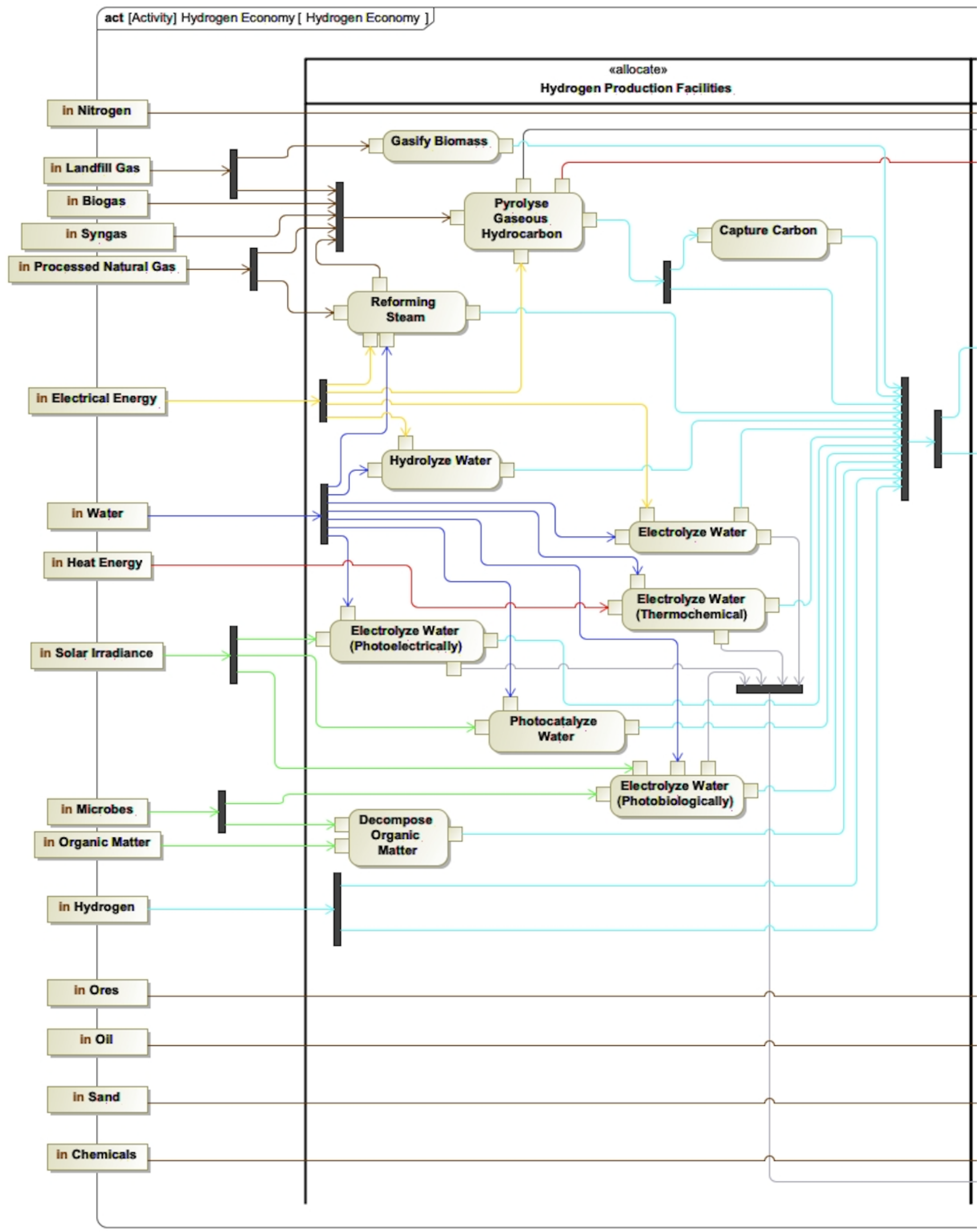

Figure 5 Hydrogen Production Activity Diagram *The model includes 11 different methods of hydrogen production and shows the inputs crossing the system boundary to supply them. See Figure A.1 in the Appendix for the full activity diagram.*

4. Hydrogen Transport and Storage

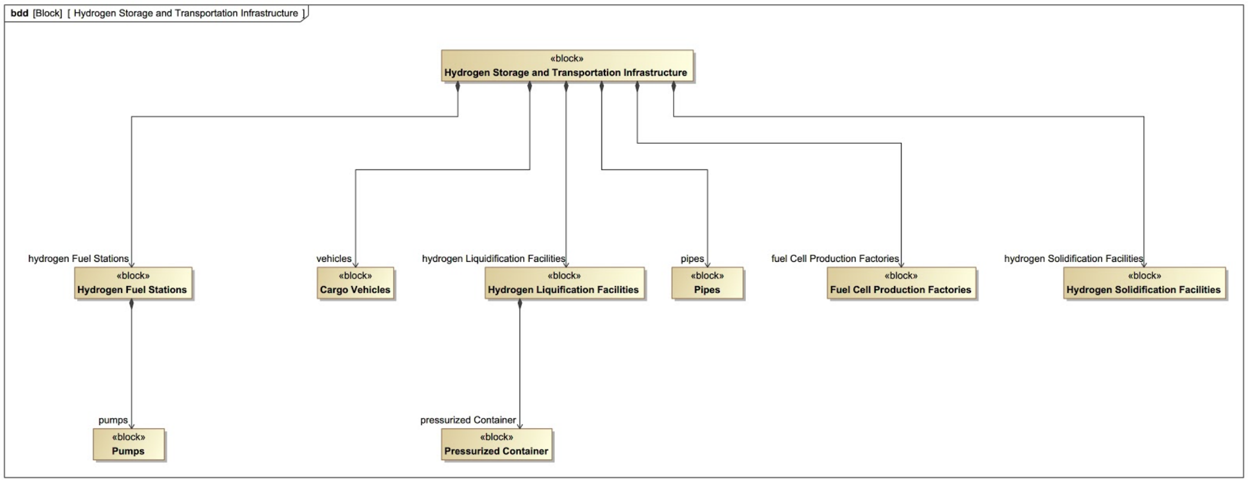

Figure 6 Hydrogen Storage and Transportation Infrastructure Block Definition Diagram *The class Hydrogen Storage and Transportation Infrastructure specializes into many different kinds of infrastructure, some of which, such as hydrogen fuel stations, depend on others.*

There are many ways of transporting hydrogen fuel from production to consumption locations (Figure 6). In its pure and gaseous form, hydrogen is extremely inefficient to transport, with an energy density of 0.01 MJ/L at 1 bar [17]. Hydrogen is transported as a gas either through pipes or freight, in pressurized shipping containers, or in pressurized shipping vehicle tanks. A dedicated hydrogen pipe system would be economical for large market and fueling station demands. When under enough pressure, hydrogen may be transported as a liquid in trucks, which is a more economical option than trucking gaseous hydrogen, but only for longer distances (for example to supply large-capacity fueling stations), because they require liquefaction facilities. Alternatively, hydrogen can be produced on site in a smaller-scale distributed fashion or in large quantities by utilities which then distribute the electricity produced by the fuel [15]. Finally, hydrogen could be made into ammonia (liquid at atmospheric pressure, 15.8 MJ/L energy density) or another derivative, which could be a solid and more easily transported [17].

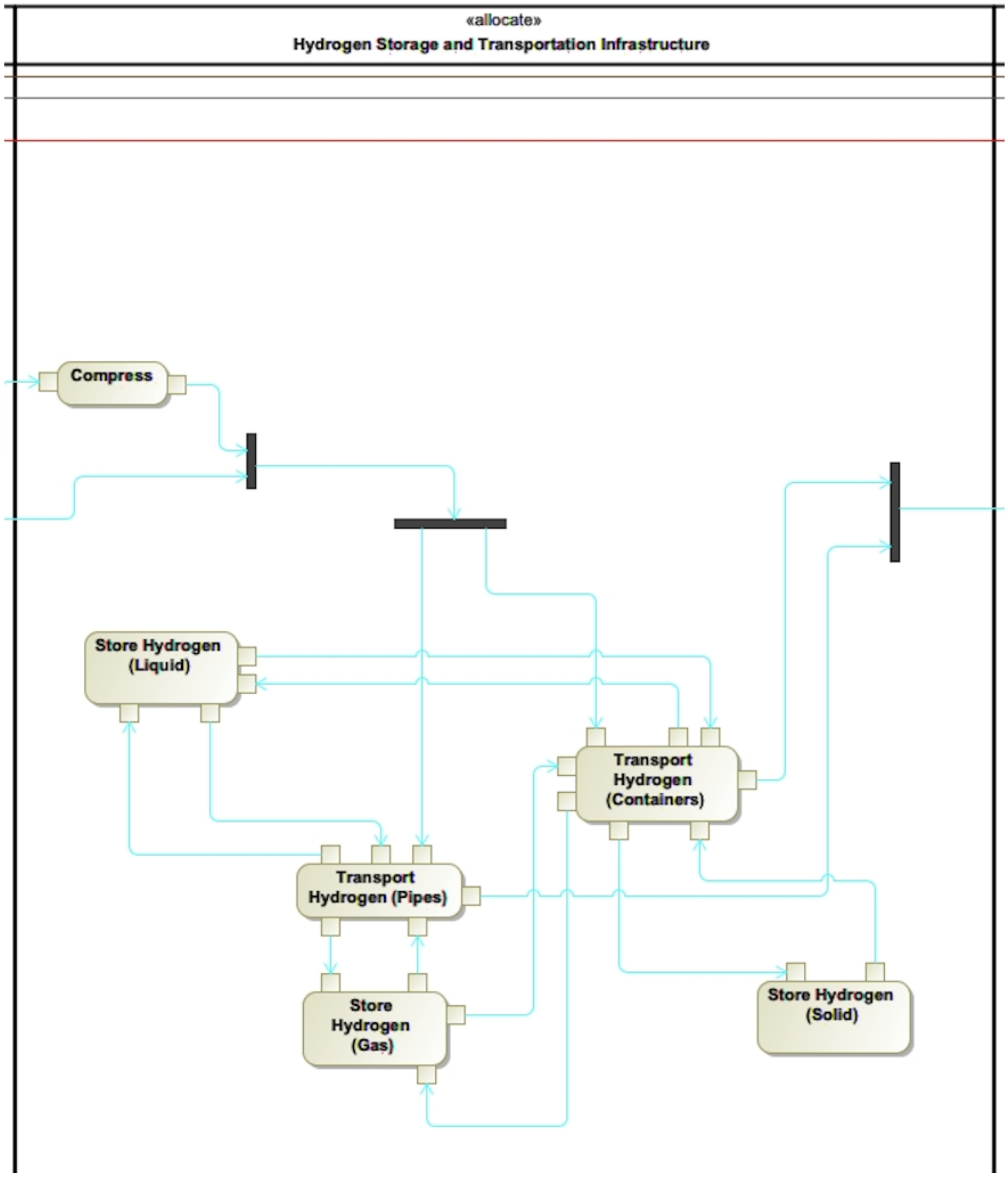

Figure 7 Hydrogen Storage and Transportation Infrastructure Activity Diagram *This snapshot of the storage and production lane of the activity model shows the various processes involved with transporting and storing hydrogen. See Figure A.1 in the Appendix for the full activity diagram.*

Another option for hydrogen distribution is to blend hydrogen into existing methane distribution pipeline systems [15]. Hydrogen fuel can be mixed into natural gas up to 5-20% by volume depending on the appliance and still be used just as natural gas would be, with no damage caused to the appliance [1]. If green hydrogen is mixed, this could decrease the emissions associated with the fuel proportionally to percent hydrogen content. This transportation method is additionally attractive because it requires minimal to no infrastructure investment and can be quickly implemented. Alternatively, hydrogen blended with natural gas can be extracted downstream at the use location by methods such as pressure swing adsorption, membrane separation, or electrochemical hydrogen separation [1]. The economic details of these technologies and the processes by which they function are beyond the scope of this report, but it is important to note that implementation of any of these extraction capabilities would require additional infrastructure and upfront investment.

Storage of hydrogen can also be tricky– gases must be stored in tight containers and take up large amounts of space. Yet again, there are many options for hydrogen storage (Figure 6). In Europe, natural and drilled salt caverns are used to store hydrogen for large consumers, such as utilities, and tanks of varying sizes offer a potentially more versatile and transportable storage mechanism. Additionally, hydrogen fueling stations offer large storage capacities, and become more economically viable as their capacity increases, although there are many factors besides size that also impact the economics of fueling stations.

5. Hydrogen Consumption

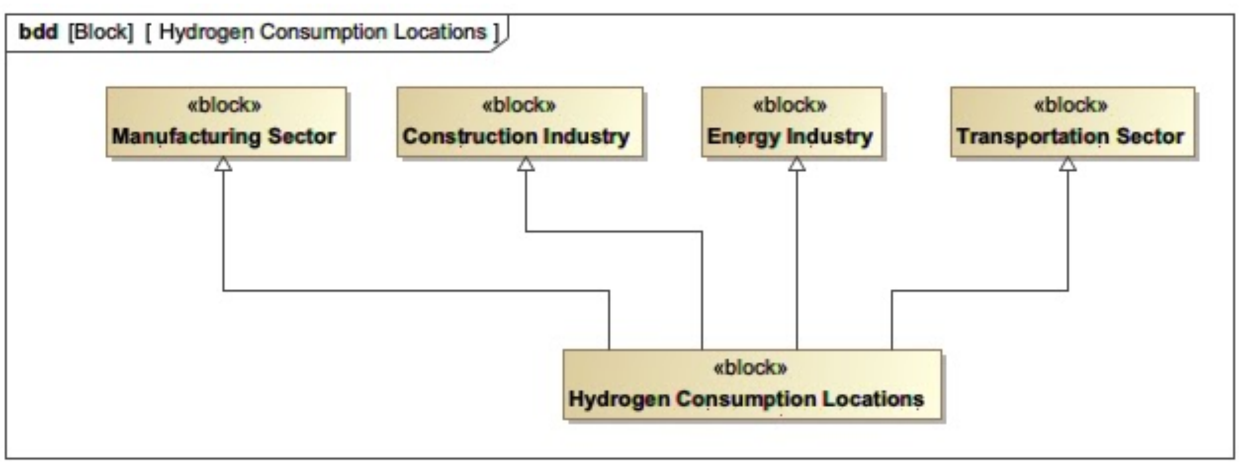

Figure 8 Hydrogen Consumption Locations Block Definition Diagram *Although there are other uses of hydrogen, for the purposes of this model, we have specialized the Hydrogen Consumption Locations Class into four subclasses: the Manufacturing Sector, the Construction Industry, the Energy Industry, and the Transportation Sector.*

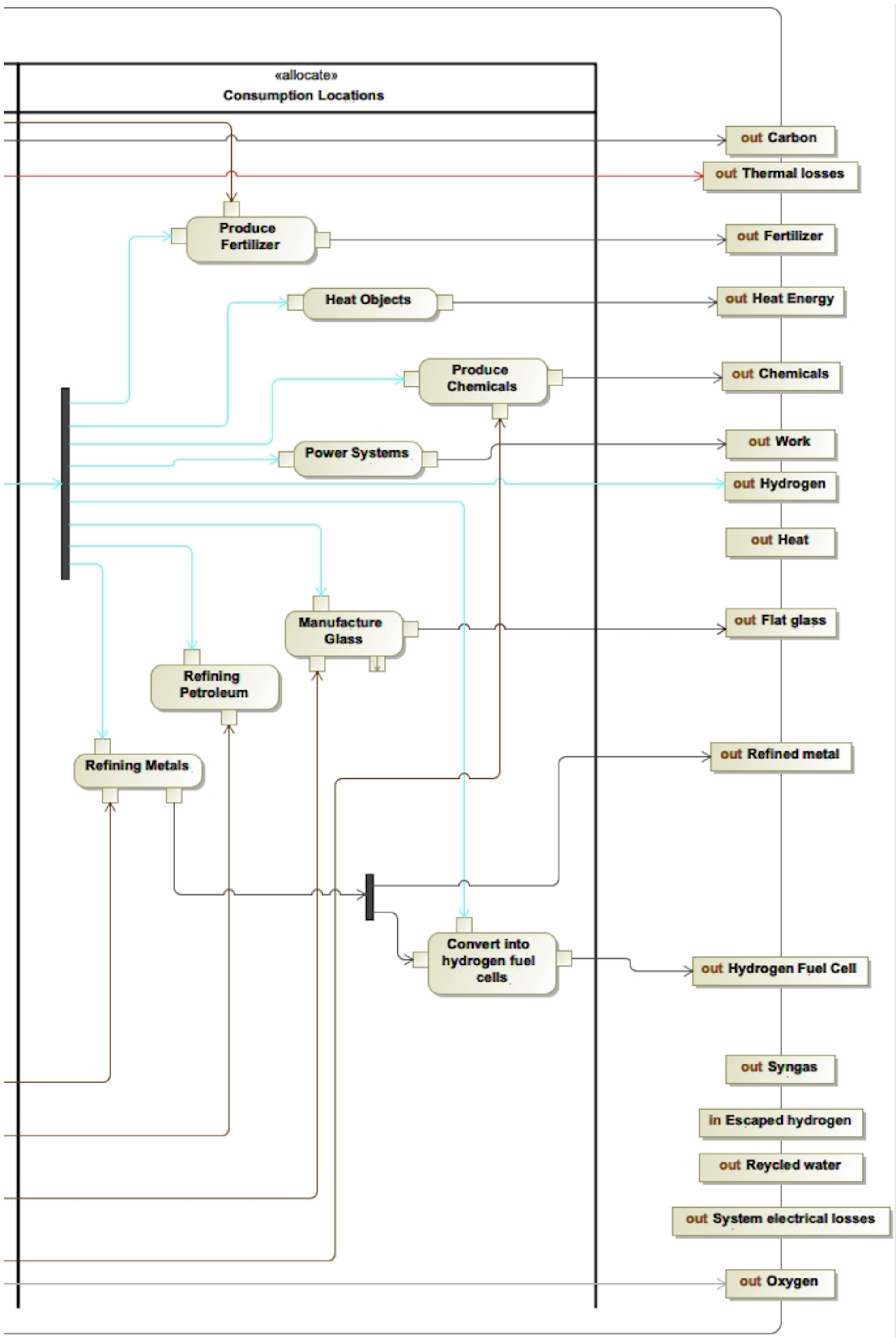

Figure 9 Hydrogen Consumption Activity Diagram *Hydrogen is primarily consumed as fuel or an ingredient in chemical or industrial production processes. This final lane of the Activity Diagram shows the outputs of the system.*

The consumption of hydrogen comes in many forms. As a fuel source, it provides relatively clean and renewable energy. As a raw material, it enables the production of fertilizers and many chemical products. As an indispensable element of refining processes, it results in cleaner petroleum and reduced metals. However, the means by which hydrogen is currently used is likely just the tip of the iceberg. Research is being conducted to explore other possible beneficial uses of hydrogen. For example, a recent trial to produce commercial-grade steel with hydrogen in place of liquified natural gas yielded successful results.

The ubiquity of hydrogen means that hydrogen is consumed at numerous locations of different sectors.

6. Hydrogen Consumption

6.1 Manufacturing Sector

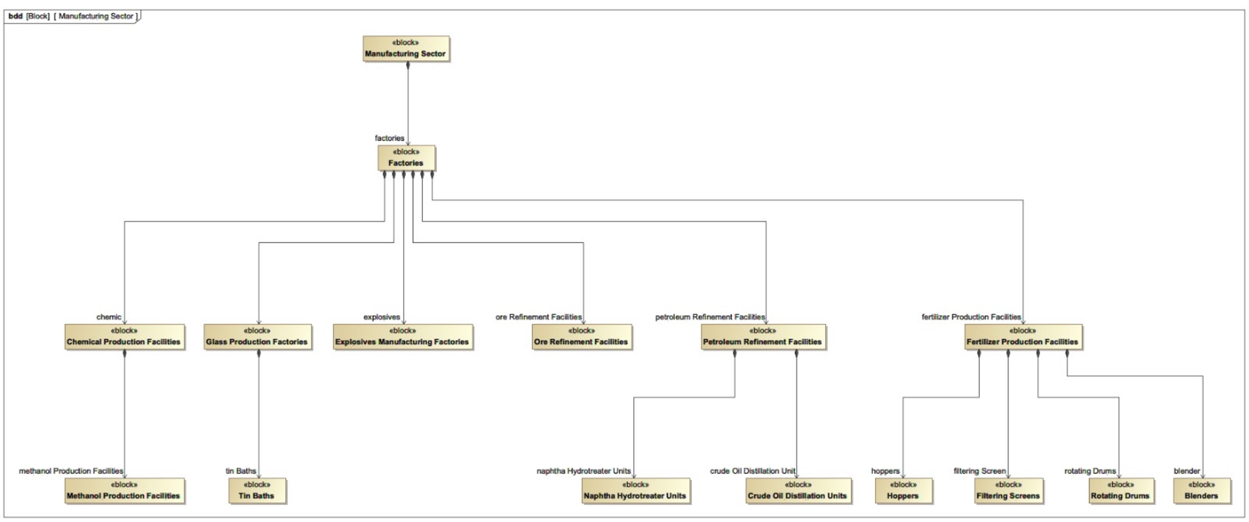

Figure 9 Hydrogen Consumption Locations: Manufacturing Sector Block Definition Diagram *The Manufacturing Sector consists of different types of factories, which use hydrogen as a chemical ingredient in their products, or as a processing agent, as is the case for Petroleum Refinement Facilities.*

In the manufacturing sector, hydrogen is utilized to produce ammonia-based fertilizer through the Haber-Bosch process, hydrochloric acid, methanol and hydrogenating agent, just to name a few. Hydrogen is also used to refine raw materials, most commonly metals and petroleum.

Environmental policies and legislations like the Clean Air Act have forced manufacturers to comply with strict measures and this will continue to grow as we face pressing deadlines to meet the different environmental challenges.

6.2 Construction Industry

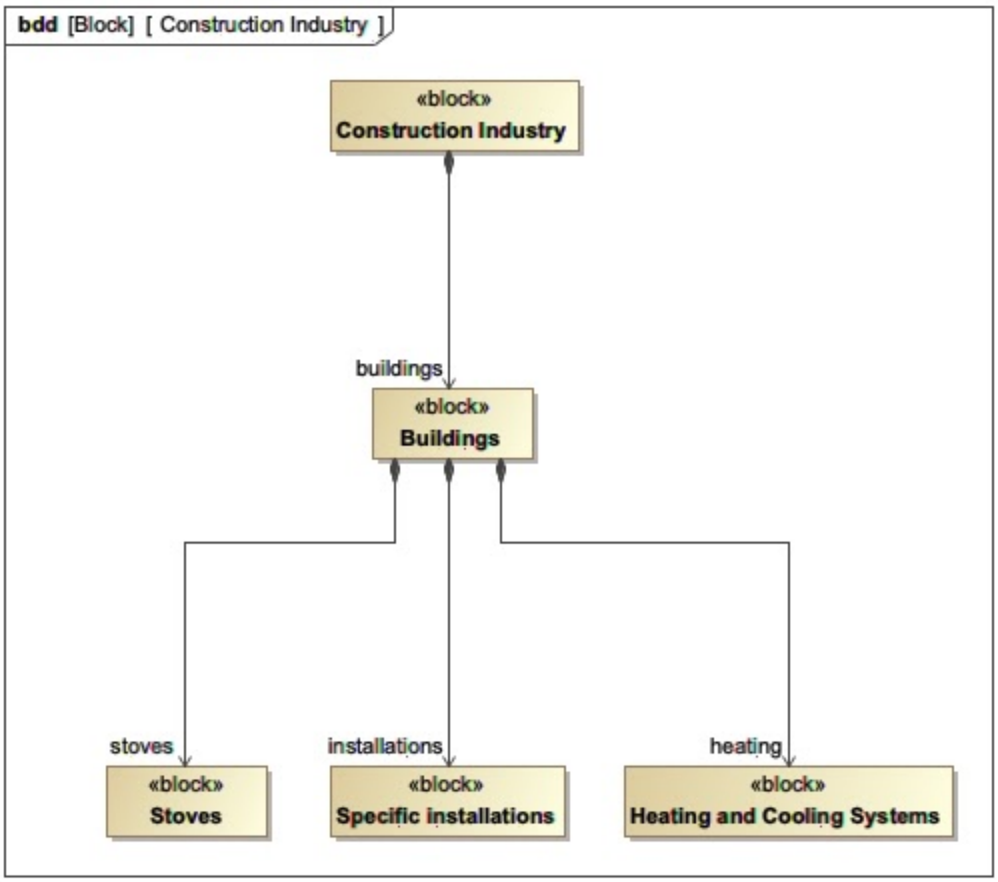

Figure 10 Hydrogen Consumption Locations: Construction Block Definition Diagram *Hydrogen use in the construction industry centers on use in complete buildings in stoves and heating and cooling systems, typically as a replacement for natural gas in appliances.*

In addition to the heating potential of hydrogen as we see with gas stoves, hydrogen is used as a coolant to cool down manufacturing plants and rockets (Schacht). Hydrogen has the highest thermal conductivity amongst all gas, with a value of 0.18W/mK. Construction industry utilize

6.3 Energy Industry

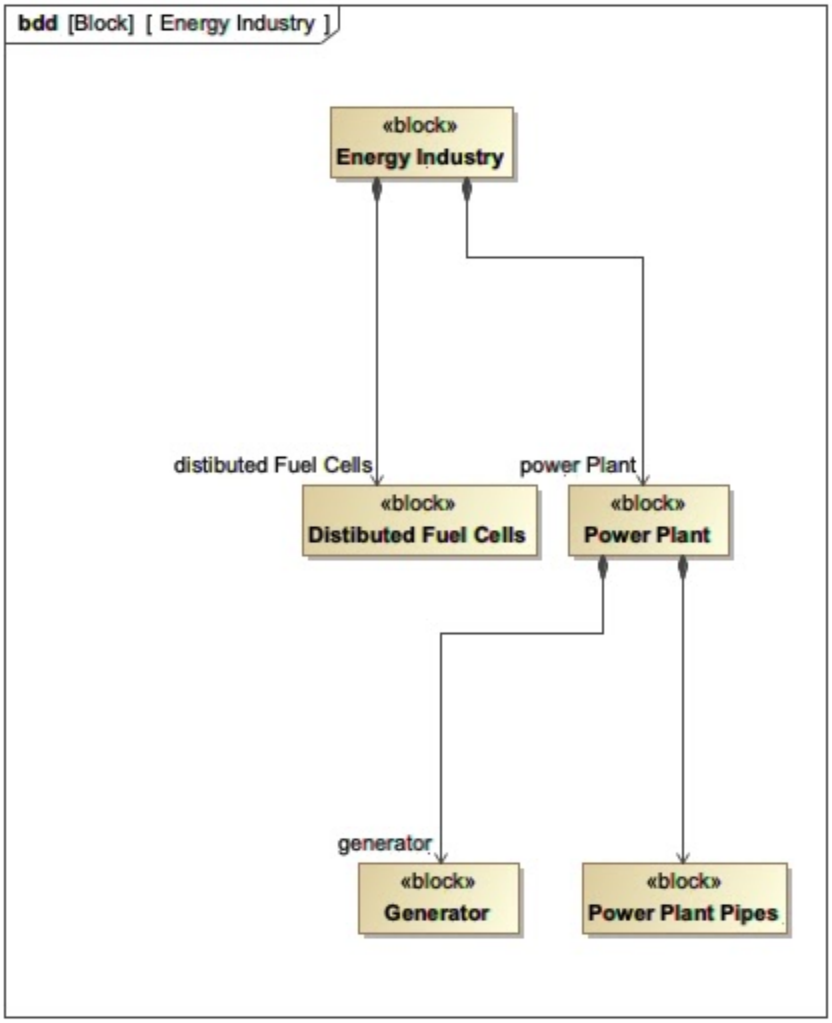

Figure 11 Hydrogen Consumption Locations: Energy Industry Block Definition Diagram *The energy industry, along with the transportation sector, is likely to be the consumption class that will grow the most as the hydrogen economy grows in the coming decades. This class specializes into distributed fuel cells for small-scale energy resiliency and power plants, operating on a utility scale.*

Hydrogen is an alternative to fossil fuels. In power plants, hydrogen reacts with oxygen to generate electricity, which will be used to power the electric grid. The attraction to use hydrogen as a replacement for fossil fuel comes from the fact that hydrogen-generated electricity produces no greenhouse gas emissions. According to the U.S. Energy Information Administration, current facilities in the U.S. has the potential to generate 250 MW of electricity as of October 2020 [19].

6.4 Transportation Sector

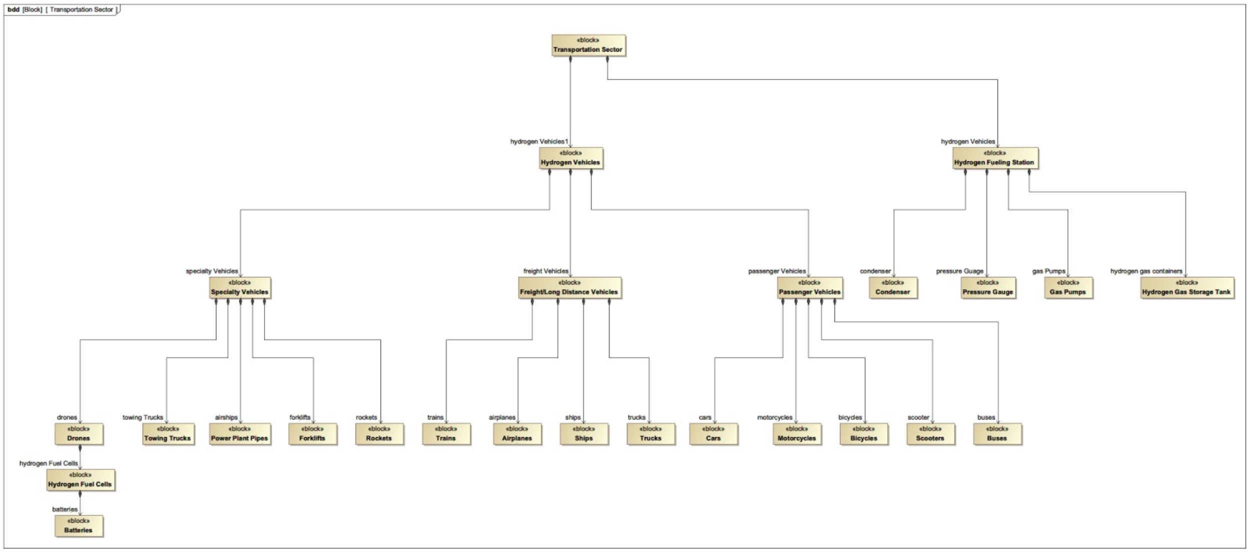

Figure 12 Hydrogen Consumption Locations: Transportation Sector Block Definition Diagram *There is much excitement about the potential of hydrogen in the Transportation Sector, and the infrastructure that must be developed is heavily interdependent for this sector to become economically viable: fueling stations are useless without hydrogen vehicles, and the inverse is also true.*

There are debates within the community as to whether hydrogen fuel cell vehicles (HFCVs) will become the prevailing type of environmentally-friendly vehicle. Some research indicates that the majority of the population prefer battery electric vehicles (BEVs). Moreover, many public figures or renowned experts in relevant fields like Elon Musk and Joseph Romm have in the past publicly stated that they do not believe in a future where HFCVs are commonly used or that HFCVs are over-hyped. However, HFCVs are generally viewed positively (Maria). This is evidenced by the increasing use of hydrogen fuel cells in the transportation sector and the continuing research efforts in advancing hydrogen fuel cell technology (Yogesh).

Similar to its application in the energy industry, hydrogen is used to power passenger vehicles, freight vehicles and specialty vehicles. While the market for hydrogen fuel cell electric vehicles is very small relative to battery electric vehicles and traditional petroleum powered vehicles, various surveys have indicated that this number will continue to grow. There are also over 25,000 forklifts powered by hydrogen in the United States in 2019 [2]. Hydrogen is also being explored for its potential to power other modes of transport like bikes, drones and scooters.

6.5 Novel Use

Hydrogen plays an increasingly important role in the medical industry where hydrogen-containing compounds have long been used in the development of drugs by pharmaceutical companies. For example, the discovery of the physiological capability of hydrogen sulfide as well as the anti-allergic and anti-inflammatory regulation ability of molecular hydrogen has opened up new avenues of treatment for certain diseases and ailments (John, [3][13]). Pending further research and official approvals by government agencies for various drugs or treatments, hydrogen may see many new applications in the medical industry that can save countless lives.

7. Network Analysis

This section analyses Hydrocity, a hypothetical instantiated architecture of an urban hydrogen economy based on the reference architecture described in our previous report (see Figures A1-A11 in the Appendix). The analysis is based both in traditional graph theory and Heterofunctional Graph Theory [20].

Hydrocity includes 26 buffers, 4 transportation resources, which represent the edges of the model, and 3 operands: we distinguish between gaseous and liquid hydrogen, and gaseous hydrogen in pressurized tanks (Figure 13). Six buffers are classified as production sites: one steam methane reforming plant, four electrolyzers, and one import dock. SMR and electrolysis are the production methods in the most advanced stages of development and most used today. The SMR plant is by far the largest producer in Hydrocity, and exclusively produces gaseous hydrogen. The electrolyzers are of varying sizes. Two are privately owned by industrial hydrogen consumers, and two others are utility-owned; these also only produce gaseous hydrogen. We wanted to additionally include the import dock to represent that Hydrocity is nested within the greater, global hydrogen economy. The import dock imports tanks of gaseous hydrogen. These six buffers are all classified as Heterofunctional Graph Theory (HFGT) transformation resources because they bring hydrogen into the system boundaries (Table 2).

These resources each perform one of two transformation processes: "produce gaseous hydrogen" or "import gaseous hydrogen."

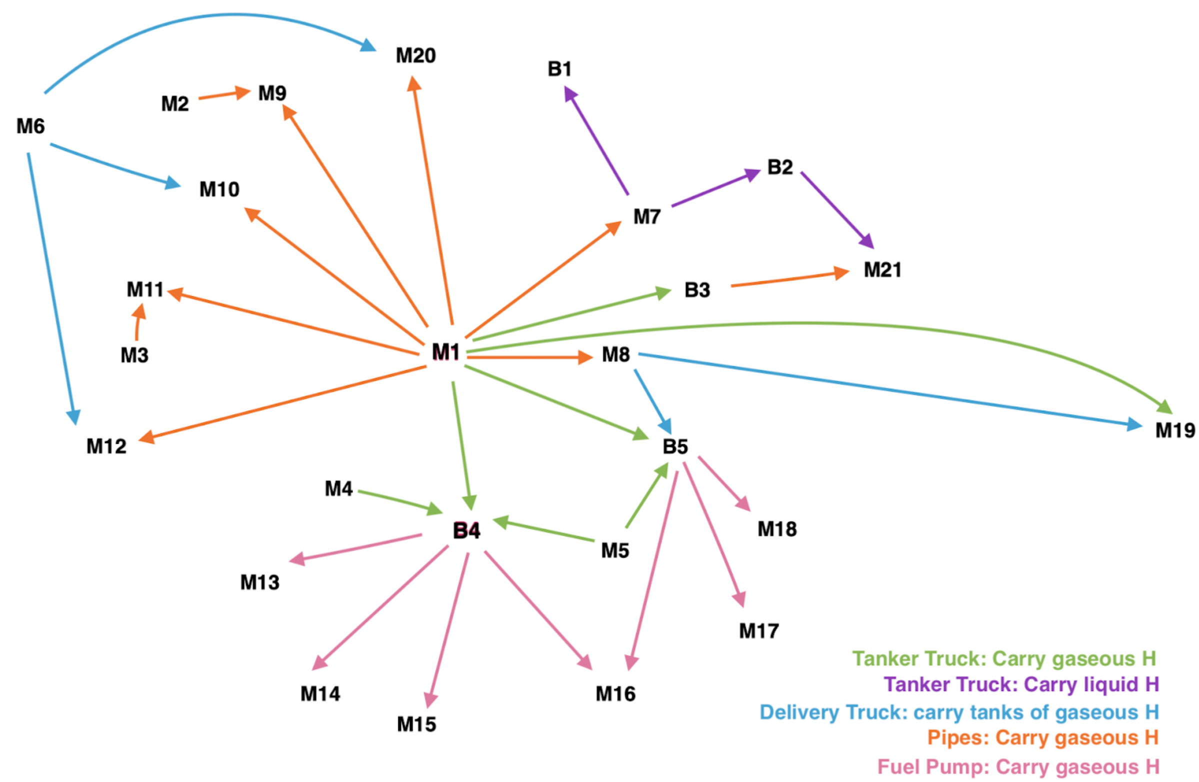

Figure 13 ***Hydrocity*** *Sketch Hydrocity is made of 26 nodes, 4 transportation resources which perform 3 different holding processes, and 3 operands.*

Model Symbol	Transformation Resource
M1	SMR Plant
M2	Electrolyzer 1
M3	Electrolyzer 2
M4	Electrolyzer 3
M5	Electrolyzer 4
M6	Import Dock
M7	Condensation Plant
M8	Tank Filling Station
M9	Ammonia Plant
M10	Metal Refinery
M11	Oil Refinery
M12	Chemical Plant
M13	Hydrogen Vehicle 1
M14	Hydrogen Vehicle 2
M15	Hydrogen Vehicle 3
M16	Hydrogen Vehicle 4
M17	Hydrogen Vehicle 5
M18	Hydrogen Vehicle 6
M19	Export Dock
M20	Syngas Plant
M21	Electricity Plant

Model Symbol	Independent Buffer
B1	Liquid Hydrogen Storage Tank 1
B2	Liquid Hydrogen Storage Tank 2
B3	Salt Cavern
B4	H Fuel Station 1
B5	H Fuel Station 2

Model Symbol	Transportation Resources
H1	Tanker Truck
H2	Delivery Truck
H3	Pipe
H4	Fuel Pump
H3	Pipe
H4	Fuel Pump

Tables 2, 3, and 4 *(From top left)*

Table 2 ***Hydrocity Transformation Resources*** *These 21 transformation resources perform any of the 8 transformation processes listed in Table 5. Together with the Independent Buffers, this is the entire model.*

Table 3 ***Hydrocity Independent Buffers*** *These 5 independent buffers store different forms of hydrogen, performing one or more of the 3 holding processes listed in Table 5. Together with the Transformation Resources, they make up the buffers of the system.*

Table 4 ***Hydrocity Transportation Resources*** *These 4 transportation resources make up the edges of the model and perform one or more of the holding processes listed in Table 5.*

Five of the nodes are classified as storage infrastructures: two liquid hydrogen storage tanks, one salt cavern, and two hydrogen fuel stations. The storage tanks serve as long-term backup storage for the eclectic grid (german-uae). The salt cavern stores gaseous hydrogen for the grid more temporarily while acting as one of its primary providers. The fuel stations hold gaseous hydrogen temporarily as well, and service hydrogen vehicles. Each of these storage infrastructures are classified as HFGT independent buffers, since no transportation nor transformation processes occur at any of them (Table 3). Two other transformation resources are involved in the transportation and storage of hydrogen: the condensation plant, which condenses the gaseous hydrogen produced by the system into liquid hydrogen, and the tank filling station, which fills pressurized tanks with gaseous hydrogen to be transported. These two transformation resources perform the processes "condense gaseous hydrogen" and "fill pressurized hydrogen tanks."

The four transportation resources in Hydrocity are (1) tanker trucks, which carry bulk gaseous and liquid hydrogen in their tanks, (2) delivery trucks, which carry tanks of gaseous hydrogen, (3) pipes, which transport gaseous hydrogen, and (4) fuel pumps, which transport gaseous hydrogen from the fuel stations to fuel cells in hydrogen vehicles (Table 4). These transportation resources, along with the independent buffers, are each capable of at least one holding process, of which there are three: carry liquid hydrogen, carry gaseous hydrogen, and carry pressurized tanks (Table 5).

Model Symbol	Transformation Process
P1	Produce H
P2	Condense H
P3	Consume gaseous H
P4	Fill H tanks
P5	Import H
P6	Export H
P7	Consume liquid H
P8	Consume H tanks
	Holding Process
G1	Carry Gaseous H
G2	Carry Liquid H
G3	Carry H tank
H3	Pipe
H4	Fuel Pump

Table 5 ***Hydrocity Processes*** *Hydrocity contains both transformation and holding processes, which serve to describe the "experience" of the operands within the system. Unless otherwise specified, the processes have gaseous hydrogen (H) as their operand.*

The final thirteen transformation resources are all sites of consumption. The operands in this system are gaseous hydrogen, liquid hydrogen, and tanks of gaseous hydrogen, therefore any process that uses one of these to provide energy, mixes any of these forms of hydrogen with other substances, or moves them across our system boundary is considered a site of consumption. In Hydrocity, there are four industrial consumption sites, including an ammonia plant, a metal refinery, an oil refinery, and a chemical plant. There are two utility consumers: an electricity plant, which uses large-scale fuel cells to turn hydrogen to electricity to be distributed by the grid, and a syngas plant, which mixes hydrogen with methane to be distributed via the methane distribution system. We included 6 hydrogen vehicles in our system; in reality there would be many, many more in order to support two hydrogen fuel stations, but for the sake of simplicity, we decided to only include six in the model. Finally, the export dock transfers hydrogen out of the system. Because these all transfer hydrogen out of the system boundary, they are considered transformation resources (Table 2). Altogether, the consumption resources perform four different transformation processes: "consume gaseous hydrogen," "consume liquid hydrogen," "consume pressurized hydrogen tanks," and "export hydrogen" (Table 5).

7.1 Formal Adjacency Matrix

	M1	M2	M3	M4	M5	M6	M7	B1	B2	B3	B4	B5	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21
M1							1			1	1	1	1	1	1	1	1							1	1	
M2														1												
M3																1										
M4											1															
M5											1	1														
M6															1		1								1	
M7								1	1																	
B1																										
B2																										1
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Figure 14 ***Inflow Adjacency Matrix*** *This matrix shows the formal connections between the transformation resources and independent buffers of Hydrocity: where there is a one, there is an inflow from the row resource to the column resource. Obviously, as all large flexible engineering systems are, this matrix and the system it represents are very sparse. The meanings of the model symbols are listed in Tables 2 and 3.*

	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	B1	B2	B3	B4	B5
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B4	1					1																				
B5									1	1																

Figure 15 ***Outflow Adjacency Matrix*** *This matrix shows the formal connections between the transformation resources and independent buffers of Hydrocity: where there is a one, there is an outflow from the column resource into the row resource. Obviously, as all large flexible engineering systems are, this matrix and the system it represents are very sparse.*

To represent the physical flows connecting transformation resources and independent buffers of the system, we made two adjacency matrices: one for the inflows of the system (Figure 14), and one for the outflows (Figure 15). These matrices are visualized in the graph in Figure 4. It is obvious just from looking at it that M1, the SMR plant, plays a central role in the system. This fact is corroborated by the Degree, Eigenvector, and Betweenness centralities of the resources (Table 7). The degree centralities are graphically represented in Figure 17. Not only does this figure and the calculated centralities show that the SMR plant is by far the most central node in the system, but they also show that the majority of resources are connected only to one or two others– a product of the production-transportation-consumption linearity of the system.

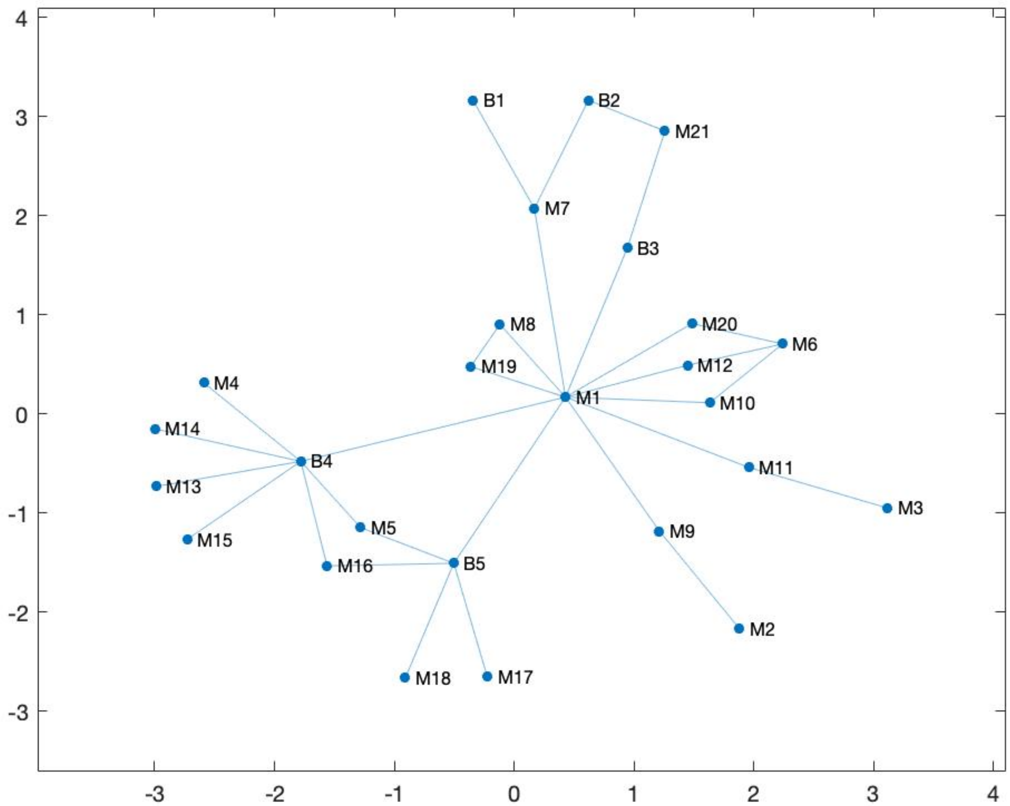

Figure 16 ***Hydrocity Digraph*** *This figure shows the directed flows of operands between nodes of Hydrocity. See Appendix for MATLAB script used to produce this.*

N	deg_cent	eig_cent	btwn
'M1'	11	0.14581	244.5
'M2'	1	0.010602	0
'M3'	1	0.010602	0
'M4'	1	0.020632	0
'M5'	2	0.038029	5
'M6'	3	0.037217	1.5
'M7'	3	0.045088	45
'M8'	2	0.051322	0
'M9'	2	0.040721	24
'M10'	2	0.04765	7.3333
'M11'	2	0.040721	24
'M12'	2	0.04765	7.3333
'M13'	1	0.020632	0
'M14'	1	0.020632	0
'M15'	1	0.020632	0
'M16'	2	0.038029	5
'M17'	1	0.017397	0
'M18'	1	0.017397	0
'M19'	2	0.051322	0
'M20'	2	0.04765	7.3333
'M21'	2	0.014968	1
'B1'	1	0.011738	0
'B2'	2	0.015635	2
'B3'	2	0.041858	21
'B4'	7	0.079248	106.5
'B5'	5	0.06682	63.5

Table 6 ***Node Centralities*** *Resource M1, the SMR plant, is by far the most central node in Hydrocity, by all centrality markers. The degree centrality counts the number of other nodes each node is connected to. The eigenvector centrality is a relative measure of the node's influence on the system. The betweenness centrality measures how often each graph node appears on a shortest path between two nodes in the graph [21].*

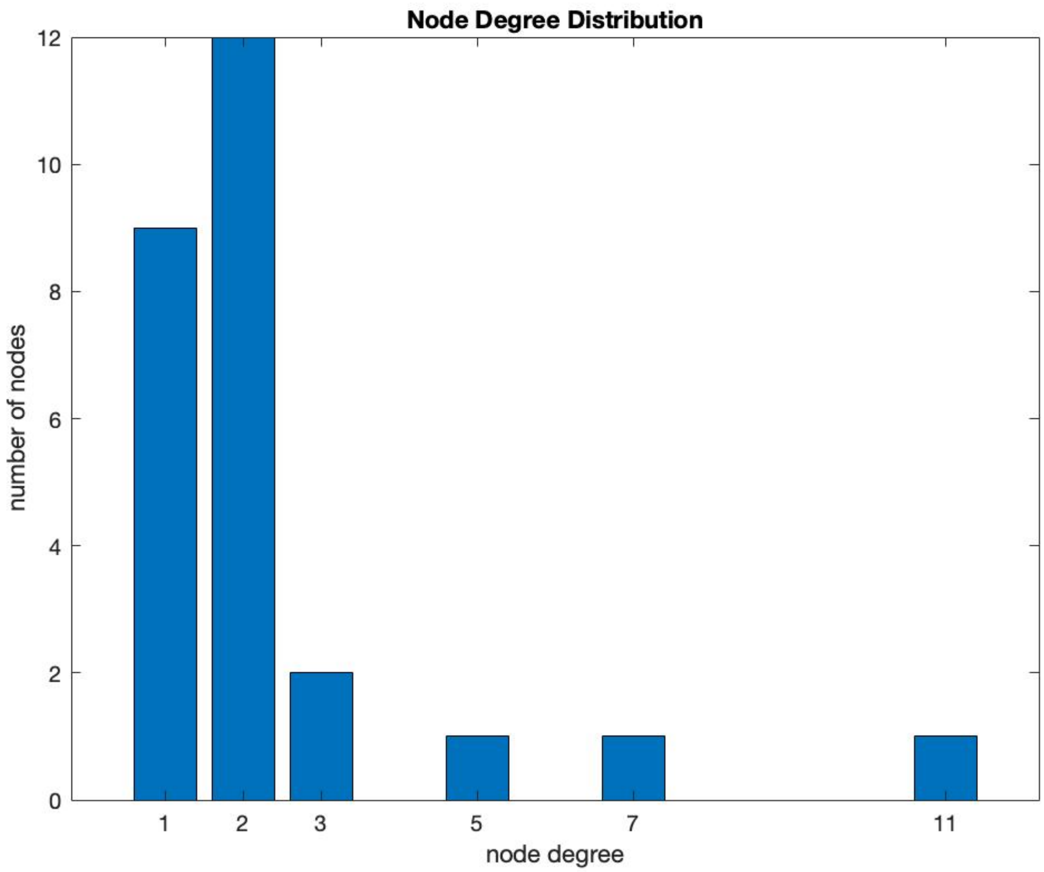

Figure 17 ***Node Degree Distribution*** *This figure plots the number of nodes against each node degree value occurring in the system; like most real physical systems, Hydrocity is made up of mostly loosely connected nodes, and relies on a few more-strongly connected nodes which act as central hubs in the system.*

7. 2 Incidence matrix

The incidence matrix shows whether an edge is linked to a node. The incidence matrix was coded up using Matlab and for a directed graph, we used 1 to represent an edge coming into a node and -1 to represent an edge going out of the node.

	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	B1	B2	B3	B4	B5
A1	-1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A2	-1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A3	-1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A4	-1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A5	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
A6	-1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A7	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
A8	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
A9	-1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A10	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
A11	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
A12	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
A13	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	-1	0
A14	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1	0
A15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-1	0
A16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	-1	0
A17	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
A18	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
A19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-1
A20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	-1
A21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-1
A22	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
A23	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
A24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	-1	0	0
A25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-1	0	0	0
A26	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
A27	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
A28	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A29	0	-1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A30	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
A31	0	0	0	0	0	-1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A32	0	0	0	0	0	-1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A33	0	0	-1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Figure 18 ***Incidence Matrix*** *This figure shows how each node and edge are connected in Hydrocity. From the incidence matrix, we can tell that the SMR plant is the central component to the system as shown by the fact that all the edges are leaving the node. It can also be seen that the hydrogen economy is like a tree where there are many areas of consumption as shown by the fact that there are many resources and buffers where only edges are coming in, but not leaving. There are some interconnecting resources and buffers as shown by the fact that some edges are coming into the resources and buffers, but also some are leaving the resources and buffers. This makes sense when looking at Figure 13.*

7. 3 Traditional Graph Theory Calculations

There are some calculations that are relevant to the traditional graph theory. The shortest path of the system from resource M1, the SMR plant, which is the central hub of the system, to a final consumption location resource M8, tank filling station, or resource M19, export dock, is 1. The longest path of the system is from resource M1, the SMR plant, to resource M21, the electricity plant, which has a length of 3. This shows that the system does not have a lot of intermediate steps to transform H after its production at the SMR plant to its consumption at the consumption location.

7.4 System Concept

The system concept is the allocation of function to form, and is represented by the matrix As, which is calculated by subtracting the System Constraints Matrix (K_s) from the System Knowledge Base (J_s). However, because our system is relatively small, we decided to instead manually construct the projected System Concept Matrix, $\tilde{A}_s$, by identifying each of the processes that actually takes place in Hydrocity and mapping them to the location at which they occur. The result (Figure 19) is a combination of the Transformation Knowledge Base (Figure 20) and the Refined Transportation Matrix (Figure 21), which itself is based on the Holding Knowledge Base (Figure 22) and the (unrefined) Transportation Knowledge Base.

The total number of degrees of freedom in each of these matrices and knowledge bases are calculated as follows:

The transformation knowledge base (Figure 20) contains a degree of freedom for each mapping of a transformation process onto a transformation resource. The transformation process *produce hydrogen* maps to 5 transformation resources and so has 5 degrees of freedom. The process *condense hydrogen* maps to one resource, producing 1 degree of freedom. The transformation process *consume gaseous hydrogen* maps to 11 transformation resources, producing 11 degrees of freedom. The processes *fill hydrogen tanks*, *import gaseous hydrogen*, *export gaseous hydrogen*, and *consume liquid hydrogen* each map to a single transformation resource, producing 1 degree of freedom each, and 4 in total. Finally, the transformation process *consume hydrogen* *tanks* maps to 4 resources, producing 4 degrees of freedom. Thus, the total number of degrees of freedom of the transformation knowledge base is 5+1+11+1+1+1+1+4 = 25 degrees of freedom.

The holding knowledge base (Figure 21) maps the holding processes onto the system resources. The process *carry gaseous hydrogen* maps to 19 transformation resources, 3 buffers, and 4 transportation resources, creating 19+3+4 = 26 degrees of freedom. The holding process *carry liquid hydrogen* maps to 2 transformation resources, 2 buffers, and one transportation resource, producing 2+2+1 = 5 degrees of freedom. Finally, the holding process *carry hydrogen tanks* maps to 4 transformation resources, 1 buffer, and 1 transportation resource, creating 4+1+1 = 6 degrees of freedom. Altogether, the holding knowledge base has 26+5+6 = 35 degrees of freedom.

The refined transportation knowledge base (Figure 22) is a combination of the holding knowledge base and the transportation knowledge base (not shown). The projected refined transportation knowledge base contains all of the realized holding process-specific transportation processes that occur within the system, and is calculated using the constraints matrix. Because of the relatively small size of Hydrocity, we manually constructed this matrix, instead of calculating it. The total number of degrees of freedom in this knowledge base is simply counted in the matrix, and comes to 65 degrees of freedom.

Finally, the number of degrees of freedom in the projected system concept matrix (Figure 7) is calculated as the sum of the degrees of freedom in the transformation process knowledge base and the projected refined transformation knowledge base: the projected system concept matrix has 25+65 = 90 degrees of freedom.

		M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	B1	B2	B3	B4	B5	H1	H2	H3	H4
P1	Produce H	1	1	1	1	1																									
P2	Condense H							1																							
P3	Consume gaseous H									1	1	1	1	1	1	1	1	1	1			1									
P4	Fill H containers								1																						
P5	Import H																														
P6	Export H																			1											
P7	Consume liquid H																					1									
P8	Consume H containers										1		1							1	1										
P9	Carry gaseous H from M1 to M7																													1	
P10	Carry gaseous H from M1 to M8																													1	
P11	Carry gaseous H from M1 to M9																													1	
P12	Carry gaseous H from M1 to M10																													1	
P13	Carry gaseous H from M1 to M11																													1	
P14	Carry gaseous H from M1 to M12																													1	
P15	Carry gaseous H from M1 to M19																											1			
P16	Carry gaseous H from M1 to M20																													1	
P17	Carry gaseous H from M1 to B3																											1			
P18	Carry gaseous H from M1 to B4																											1			
P19	Carry gaseous H from M1 to B5																											1			
P20	Carry gaseous H from M4 to B4																											1			
P21	Carry gaseous H from M5 to B4																											1			
P22	Carry gaseous H from M5 to B5																											1			
P23	Carry gaseous H from B3 to M21																													1	
P24	Carry gaseous H from M2 to M9																													1	
P25	Carry gaseous H from M3 to M11																													1	
P26	Store gaseous H at B3																								1						
P27	Store gaseous H at B4																									1					
P28	Store gaseous H at B5																										1				
P29	Carry gaseous H from B4 to M13																														1
P30	Carry gaseous H from B4 to M14																														1
P31	Carry gaseous H from B4 to M15																														1
P32	Carry gaseous H from B4 to M16																														1
P33	Carry gaseous H from B5 to M16																														1
P34	Carry gaseous H from B5 to M17																														1
P35	Carry gaseous H from B5 to M18																														1
P36	Carry liquid H from M7 to B1																											1			
P37	Carry liquid H from M7 to B2																											1			
P38	Carry liquid H from B2 to M21																											1			
P39	Store liquid H at B1																						1								
P40	Store liquid H at B2																							1							
P41	Carry H tanks from M6 to M20																												1		
P42	Carry H tanks from M6 to M10																												1		
P43	Carry H tanks from M6 to M12																												1		
P44	Carry H tanks from M8 to B5																												1		
P45	Carry H tanks from M8 to M19																												1		
P46	Store gaseous H at M1	1																													
P47	Store gaseous H at M2		1																												
P48	Store gaseous H at M3			1																											
P49	Store gaseous H at M4				1																										
P50	Store gaseous H at M5					1																									
P51	Store gaseous H at M6						1																								
P52	Store gaseous H at M7							1																							
P53	Store gaseous H at M8								1																						
P54	Store gaseous H at M9									1																					
P55	Store gaseous H at M10										1																				
P56	Store gaseous H at M11											1																			
P57	Store gaseous H at M12												1																		
P58	Store gaseous H at M13													1																	
P59	Store gaseous H at M14														1																
P60	Store gaseous H at M15															1															
P61	Store gaseous H at M16																1														
P62	Store gaseous H at M17																	1													
P63	Store gaseous H at M18																		1												
P64	Store gaseous H at M19																			1											
P65	Store gaseous H at M20																				1										
P66	Store gaseous H at M21																					1									
P67	Store H tanks at M8								1																						
P68	Store H tanks at M10										1																				
P69	Store H tanks at M12												1																		
P70	Store H tanks at M19																			1											
P71	Store H tanks at M20																				1										
P72	Store H tanks at B5																										1				
P73	Store liquid H at M21																					1									

Figure 19 ***Projected System Concept Matrix*** *As expected, even the projected version of the system concept matrix is sparse. Its total size is 73x30, meaning there are 2,190 possible connections, of which 90, or 4.11%, are realized degrees of freedom in Hydrocity.*

		M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21
Produce H	P1	1	1	1	1	1																
Condense H	P2							1														
Consume gaseous H	P3									1	1	1	1	1	1	1	1	1	1			1
Fill H tanks	P4								1													
Import H	P5						1															
Export H	P6																			1		
Consume liquid H	P7																					1
Consume H tanks	P8										1		1							1	1	

Figure 20 ***Transformation Knowledge Base*** *The Transformation Knowledge Base assigns transformation processes to those resources which can complete them. Hydrocity's transformation knowledge base contains 25 degrees of freedom. The 8 processes and 21 resources associated with transformation are identified and matched to their model symbols in Tables 4 and 1, respectively.*

	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	B1	B2	B3	B4	B5	H1	H2	H3	H4
Carry gaseous H from M1 to M7																														1	
Carry gaseous H from M1 to M8																														1	
Carry gaseous H from M1 to M9																														1	
Carry gaseous H from M1 to M10																														1	
Carry gaseous H from M1 to M11																														1	
Carry gaseous H from M1 to M12																														1	
Carry gaseous H from M1 to M19																												1			
Carry gaseous H from M1 to M20																														1	
Carry gaseous H from M1 to B3																												1			
Carry gaseous H from M1 to B4																												1			
Carry gaseous H from M1 to B5																												1			
Carry gaseous H from M4 to B4																												1			
Carry gaseous H from M5 to B4																												1			
Carry gaseous H from M5 to B5																												1			
Carry gaseous H from B3 to M21																														1	
Carry gaseous H from M2 to M9																														1	
Carry gaseous H from M3 to M11																														1	
Store gaseous H at B3																									1						
Store gaseous H at B4																										1					
Store gaseous H at B5																											1				
Carry gaseous H from B4 to M13																															1
Carry gaseous H from B4 to M14																															1
Carry gaseous H from B4 to M15																															1
Carry gaseous H from B4 to M16																															1
Carry gaseous H from B5 to M16																															1
Carry gaseous H from B5 to M17																															1
Carry gaseous H from B5 to M18																															1
Carry liquid H from M7 to B1																												1			
Carry liquid H from M7 to B2																												1			
Carry liquid H from B2 to M21																												1			
Store liquid H at B1																							1								
Store liquid H at B2																								1							
Carry H tanks from M6 to M20																													1		
Carry H tanks from M6 to M10																													1		
Carry H tanks from M6 to M12																													1		
Carry H tanks from M8 to B5																													1		
Carry H tanks from M8 to M19																													1		
Store gaseous H at M1	1																													
Store gaseous H at M2		1																												
Store gaseous H at M3			1																											
Store gaseous H at M4				1																										
Store gaseous H at M5					1																									
Store gaseous H at M6						1																								
Store gaseous H at M7							1																							
Store gaseous H at M8								1																						
Store gaseous H at M9									1																					
Store gaseous H at M10										1																				
Store gaseous H at M11											1																			
Store gaseous H at M12												1																		
Store gaseous H at M13													1																	
Store gaseous H at M14														1																
Store gaseous H at M15															1															
Store gaseous H at M16																1														
Store gaseous H at M17																	1													
Store gaseous H at M18																		1												
Store gaseous H at M19																			1											
Store gaseous H at M20																				1										
Store gaseous H at M21																					1									
Store H tanks at M8								1																						
Store H tanks at M10										1																				
Store H tanks at M12												1																		
Store H tanks at M19																			1											
Store H tanks at M20																				1										
Store H tanks at B5																											1				
Store liquid H at M21																					1									
Store liquid H at M7							1																							

Figure 21 ***Refined Transportation Knowledge Base*** *This matrix assigns transportation processes to the transformation resources, buffers, and holding resources that can perform each. The holding resources are those*

that perform the most transportation processes of any of the resources and buffers. The refined transportation knowledge base contains 66 degrees of freedom.

		M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	B1	B2	B3	B4	B5	H1	H2	H3	H4	H5
Carry Gaseous H	G1	1	1	1	1	1	1			1	1	1	1	1	1	1	1	1	1	1	1	1			1	1	1	1		1	1	1
Carry Liquid H	G2							1	1														1	1				1				
Carry H tank	G3										1		1							1	1						1		1			

Figure 22 ***Holding Knowledge Base*** *This matrix matches the holding processes, of which there are 3, to each of the transformation resources, buffers, and holding resources that can perform them. The names of the resources and buffers may be found in Tables 1, 2, and 3.*

7. 5 Heterofunctional Adjacency Matrix

Figure 23 ***Heterofunctional adjacency matrix*** *The heterofunctional adjacency matrix is a representation of function to form. The heterofunctional adjacency matrix tells us more information about the system than the traditional adjacency matrix because it shows how the formal element of the entire system is connected with each other in a*

given way. Like the traditional adjacency matrix, we can tell that the consumption locations and the export dock are the locations for the output of the system and the production facilities as well as the import dock are the locations for the input of the system. However, with the heterofunctional adjacency matrix, we can also for example tell that the SMR plant in Hydrocity is connected with H fuel station 1 and H fuel station 2 through liquid tanker trucks. There are no pipes or delivery trucks connecting the SMR plant with H fuel station 1 and H fuel station 2 so immediately we know more about the system. The meanings of the column and row labels are shown in Figure 12.

	Process		Process
1	Produce H at SMR plant	46	Carry gaseous H from H fuel station 1 to hydrogen vehicle 4 with fuel pump
2	Produce H at electrolyzer 1	47	Carry gaseous H from H fuel station 2 to hydrogen vehicle 4 with fuel pump
3	Produce H at electrolyzer 2	48	Carry gaseous H from H fuel station 2 to hydrogen vehicle 5 with fuel pump
4	Produce H at electrolyzer 3	49	Carry gaseous H from H fuel station 2 to hydrogen vehicle 6 with fuel pump
5	Produce H at electrolyzer 4	50	Carry liquid H from condensation plant to liquid hydrogen storage tank 1 with tanker truck
6	Condense H to produce liquid H at condenser plant	51	Carry liquid H from condensation plant to liquid hydrogen storage tank 2 with tanker truck
7	Consume gaseous H at ammonia plant	52	Carry liquid H from liquid hydrogen storage tank 2 to electricity plant with tanker truck
8	Consume gaseous H at metal refinery	53	Carry H tanks from import dock to syngas plant with delivery truck
9	Consume gaseous H at oil refinery	54	Carry H tanks from import dock to metal refinery with delivery truck
10	Consume gaseous H at chemical plant	55	Carry H tanks from import dock to chemical plant with delivery truck
11	Consume gaseous H at hydrogen vehicle 1	56	Carry H tanks from tank filling station to H fuel station 2 with delivery truck
12	Consume gaseous H at hydrogen vehicle 2	57	Carry H tanks from tank filling station to export dock with delivery truck
13	Consume gaseous H at hydrogen vehicle 3	58	Store gaseous H at salt cavern
14	Consume gaseous H at hydrogen vehicle 4	59	Store gaseous H at H fuel station 1
15	Consume gaseous H at hydrogen vehicle 5	60	Store gaseous H at H fuel station 2
16	Consume gaseous H at hydrogen vehicle 6	61	Store liquid H at liquid storage tank 1
17	Consume gaseous H at electricity plant	62	Store liquid H at liquid storage tank 2
18	Fill H tank at tank filling station	63	Store gaseous H at SMR plant
19	Import H at Import Dock	64	Store gaseous H at electrolyzer 1
20	Export H at export dock	65	Store gaseous H at electrolyzer 2
21	Consume liquid H at electricity plant	66	Store gaseous H at electrolyzer 3
22	Consume H tank at metal refinery	67	Store gaseous H at electrolyzer 4
23	Consume H tank at chemical plant	68	Store gaseous H at import dock
24	Export H tank at export dock	69	Store gaseous H at condensation plant
25	Consume H tank at syngas plant	70	Store gaseous H at tank filling station
26	Carry gaseous H from SMR plant to condensation plant with pipe	71	Store gaseous H at ammonia plant
27	Carry gaseous H from SMR plant to tank filling station with pipe	72	Store gaseous H at metal refinery
28	Carry gaseous H from SMR plant to ammonia plant with pipe	73	Store gaseous H at oil refinery
29	Carry gaseous H from SMR plant to metal refinery with pipe	74	Store gaseous H at chemical plant
30	Carry gaseous H from SMR plant to oil refinery with pipe	75	Store gaseous H at hydrogen vehicle 1
31	Carry gaseous H from SMR plant to chemical plant with pipe	76	Store gaseous H at hydrogen vehicle 2
32	Carry gaseous H from SMR plant to export dock with pipe	77	Store gaseous H at hydrogen vehicle 3
33	Carry gaseous H from SMR plant to syngas plant with tanker truck	78	Store gaseous H at hydrogen vehicle 4
34	Carry gaseous H from SMR plant to salt cavern with pipe	79	Store gaseous H at hydrogen vehicle 5
35	Carry gaseous H from SMR plant to H fuel station 1 with tanker truck	80	Store gaseous H at hydrogen vehicle 6
36	Carry gaseous H from SMR plant to H fuel station 2 with tanker truck	81	Store gaseous H at export dock
37	Carry gaseous H from electrolyzer 3 to H fuel station 1 with tanker truck	82	Store gaseous H at syngas plant
38	Carry gaseous H from electrolyzer 4 to H fuel station 1 with tanker truck	83	Store gaseous H at electricity plant
39	Carry gaseous H from electrolyzer 4 to H fuel station 2 with tanker truck	84	Store H tanks at tank filling station
40	Carry gaseous H from salt cavern to electricity plant with pipe	85	Store H tanks at metal refinery
41	Carry gaseous H from electrolyzer 1 to ammonia plant with pipe	86	Store H tanks at chemical plant
42	Carry gaseous H from electrolyzer 2 to oil refinery with pipe	87	Store H tanks at export dock
43	Carry gaseous H from H fuel station 1 to hydrogen vehicle 1 with fuel pump	88	Store H tanks at syngas plant
44	Carry gaseous H from H fuel station 1 to hydrogen vehicle 2 with fuel pump	89	Store H tanks at H fuel station 2
45	Carry gaseous H from H fuel station 1 to hydrogen vehicle 3 with fuel pump	90	Store liquid H at electricity plant
		91	Store liquid H at condensation plant

Figure 24 ***Heterofunctional Adjacency Matrix Legend***

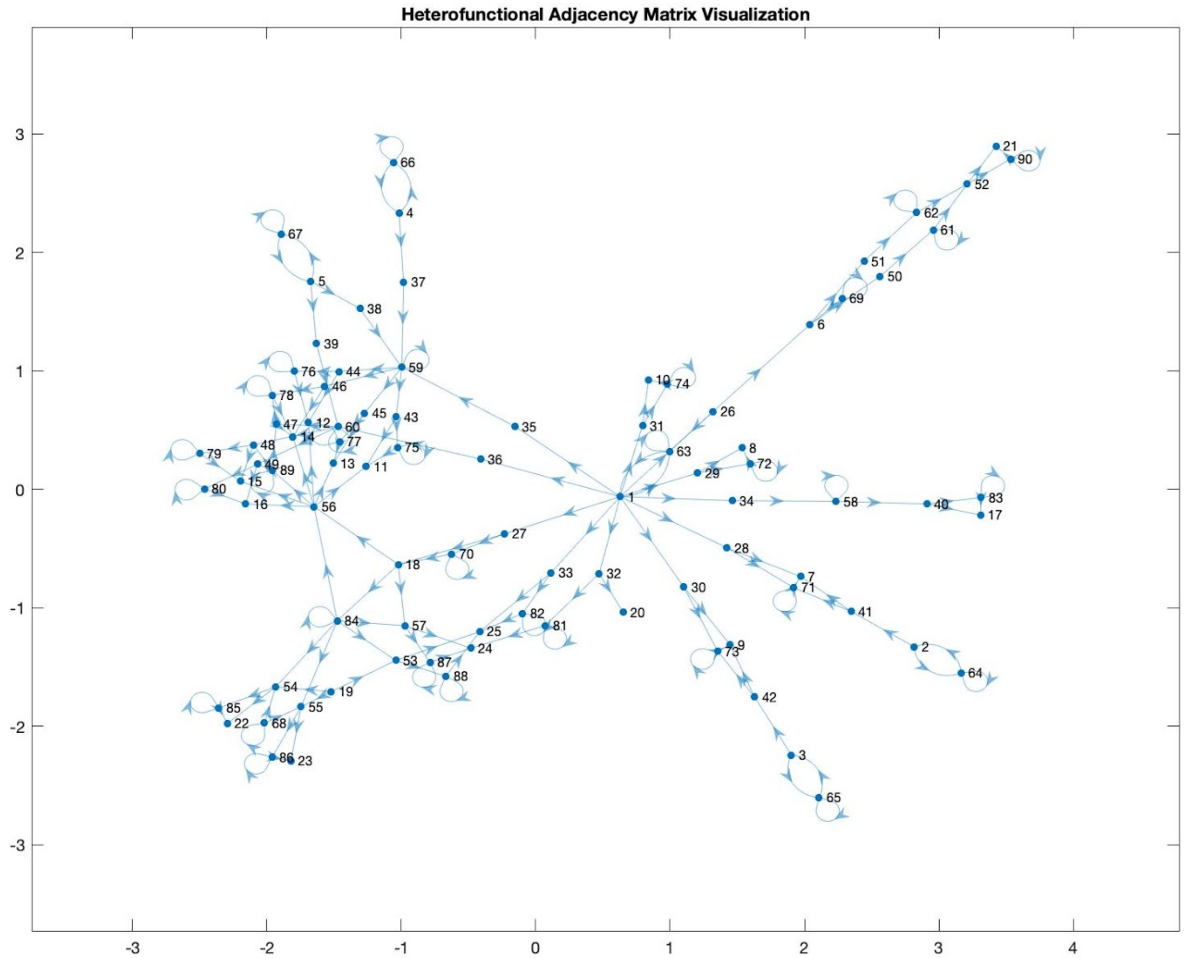

Figure 25 ***Hydrocity Heterofunctional Digraph*** *This figure shows the directed flows of operands between nodes of Hydrocity from a heterofunctional graph theory point of view. This digraph provides more information as compared to the digraph drawn from a traditional graph theory point of view as we can tell since there are more nodes and processes in the digraph so even though we are analysing the same system, we can learn more about the system with heterofunctional graph theory.*

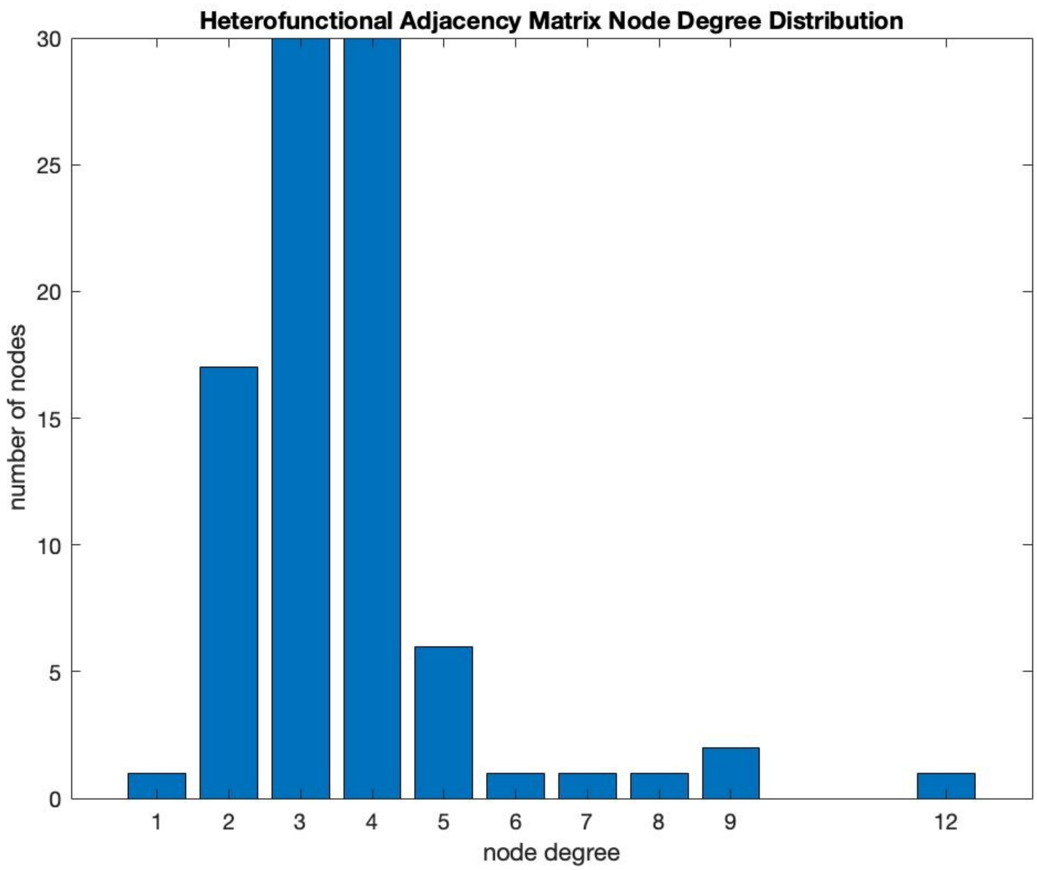

Figure 26 ***Heterofunctional Adjacency Matrix Node Degree Distribution*** *This figure plots the number of nodes against each node degree value occurring in the system for the heterofunctional adjacency matrix; most nodes are connected with 2 to 4 nodes with a few nodes that have even greater node connections. It shows that Hydrocity is a well connected system with a few center hubs. The number of nodes each node is on average connected to, indicate greater connections than Figure 5, which is the same figure but for traditional adjacency matrix. This shows that the heterogeneity of the system is so strong that some connections are missed in the traditional adjacency matrix but is shown in the heterofunctional adjacency matrix.*

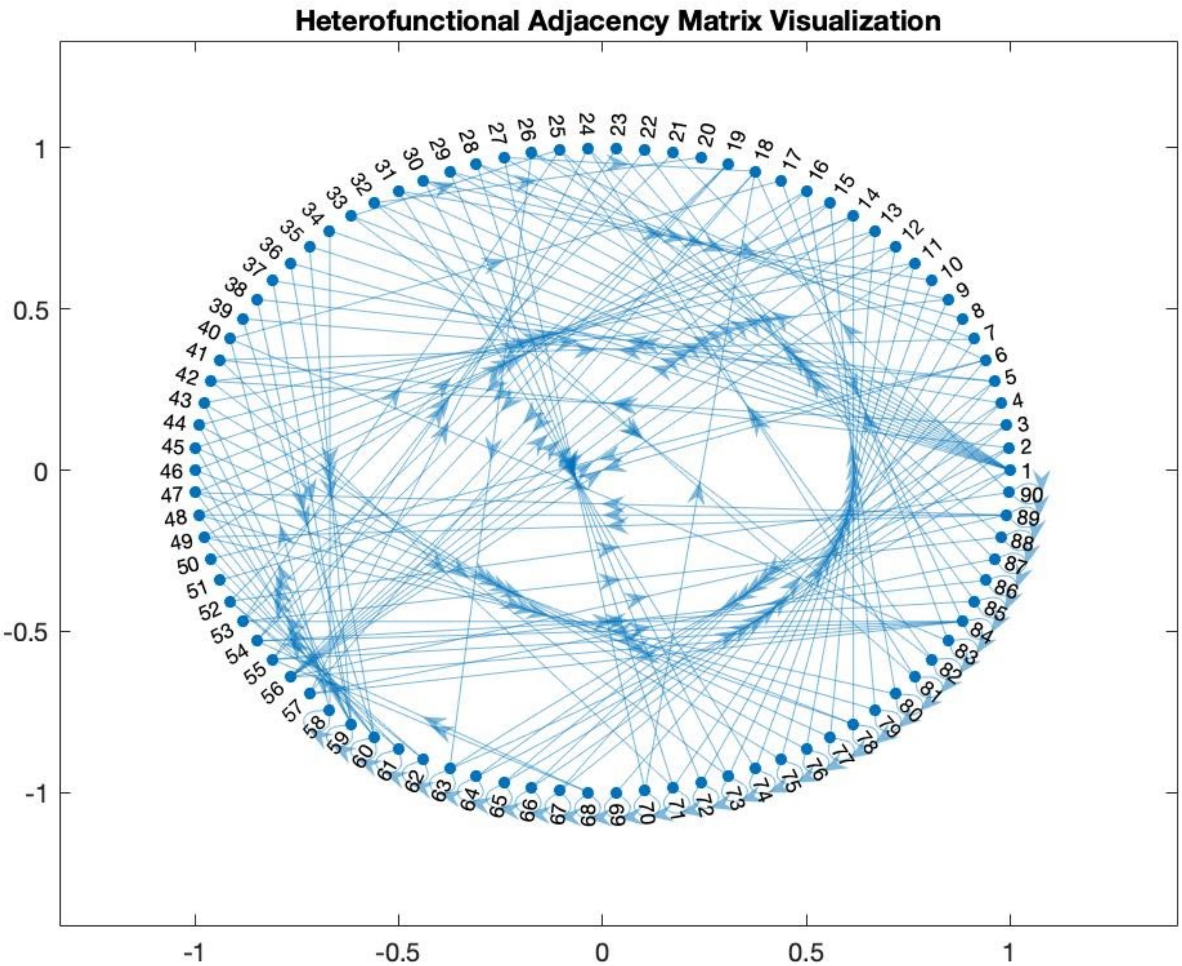

Figure 27 ***Heterofunctional Adjacency Matrix*** *This is a visualization of the heterofunctional adjacency matrix that shows the many connections between each node. There are 168 connections in the system, which shows the complexity of the system so it is very important to manage the complexity well.*

DOF	Degree Centrality	Eigenvector Centrality	Betweenness Centrality	DOF	Degree Centrality	Eigenvector Centrality	Betweenness Centrality
1	12	0.025503	2698.9	46	3	0.015568	92.613
2	2	0.00035732	89	47	4	0.026026	88.178
3	2	0.00035732	89	48	4	0.023061	107.74
4	2	0.0011721	89	49	4	0.023061	107.74
5	3	0.0029137	109.7	50	3	0.0011631	210.67
6	5	0.003105	738.17	51	3	0.0011631	210.67
7	3	0.002731	129	52	4	0.00022077	177.67
8	2	0.0021803	0	53	4	0.02173	155.86
9	3	0.002731	129	54	5	0.024275	230.46
10	2	0.0021803	0	55	5	0.024275	230.46
11	3	0.018201	87.405	56	9	0.060904	764.15
12	3	0.018201	87.405	57	4	0.027973	133.19
13	3	0.018201	87.405	58	4	0.0020028	261
14	4	0.027982	109.86	59	9	0.019955	856.33
15	3	0.022131	61.706	60	7	0.026736	497.1
16	3	0.022131	61.706	61	4	0.00040756	129.33
17	2	0.00017123	0	62	4	0.00040756	129.33
18	5	0.042323	643.13	63	4	0.010105	0
19	3	0.015989	20.5	64	3	0.00010524	0
20	1	0.0016724	0	65	3	0.00010524	0
21	2	6.969e-05	0	66	3	0.0003452	0
22	2	0.0076627	0	67	3	0.00085812	0
23	2	0.0076627	0	68	4	0.014299	3
24	3	0.010082	57.976	69	3	0.00091448	0
25	4	0.010649	171.52	70	4	0.018231	0
26	3	0.0088075	800	71	5	0.0033523	129
27	3	0.019579	625.59	72	4	0.0026764	0
28	3	0.0071861	425	73	5	0.0033523	129
29	3	0.0069071	176	74	4	0.0026764	0
30	3	0.0071861	425	75	4	0.0084859	0
31	3	0.0069071	176	76	4	0.0084859	0
32	3	0.0073507	218.81	77	4	0.0084859	0
33	3	0.0095802	249.9	78	5	0.020491	9.404
34	2	0.0062578	344	79	4	0.01331	0
35	2	0.010342	672.17	80	4	0.01331	0
36	2	0.011885	453.54	81	4	0.0051343	82.643
37	2	0.0048066	176	82	4	0.0059577	0
38	2	0.0052028	102.46	83	4	0.00021018	0
39	2	0.0067457	93.107	84	8	0.059339	743.21
40	3	0.00054243	176	85	4	0.0094061	0
41	3	0.0014653	176	86	4	0.0094061	0
42	3	0.0014653	176	87	4	0.011208	0
43	3	0.010612	109.57	88	4	0.0095361	0
44	3	0.010612	109.57	89	6	0.039186	81.368
45	3	0.010612	109.57	90	4	8.5545e-05	0
				91	5	0.0015996	1.1667

Table 7 ***Node Centralities*** *The node centralities of the heterofunctional adjacency matrix show similar information to the node centralities of the traditional adjacency matrix. Resource M1, the SMR plant, is by far the most central node in Hydrocity, by all centrality markers. The degree centrality counts the number of other nodes each node is connected to. The eigenvector centrality is a relative measure of the node's influence on the system. The betweenness*

centrality measures how often each graph node appears on a shortest path between two nodes in the graph and is calculated with [20]. However, we also see new information with the node centralities of the heterofunctional adjacency matrix. There are several nodes with high node centralities like M84 which is Store H tanks in tank filling stations. This shows the heterogeneity of the system is great.

8. Hydrocity Service Net

The hydrogen economy of Hydrocity functions to provide one service: provide hydrogen to consumers. This hydrogen takes three forms, the operands of the system, which are gaseous hydrogen, liquid hydrogen, and tanks of gaseous hydrogen. The basic service system is modeled with a Petri Net (Figure 28). The places of the service net (circles) represent the three operand states of hydrogen (the service), and the transitions (boxes) represent processes that happen to the hydrogen.

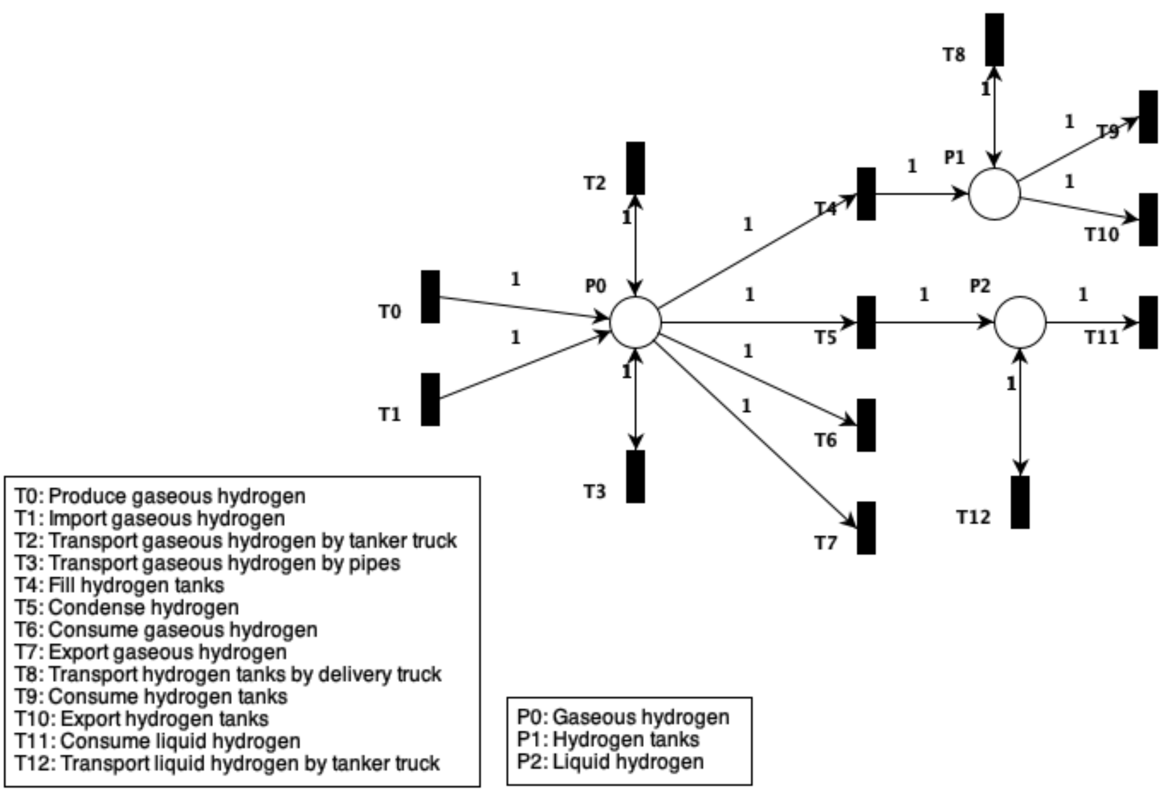

Figure 28 ***Hydrocity Service Net*** *The service net shows a lot of information about Hydrocity. We see that the system is very heterogeneous. There are three forms of hydrogen in Hydrocity gaseous hydrogen, hydrogen tanks, and liquid hydrogen. We see that gaseous hydrogen is the major form of hydrogen in Hydrocity. In addition to its use for consumption, it also acts as input to both filling hydrogen tanks and condensing hydrogen into liquid hydrogen. Each type of hydrogen is used differently. For example, liquid hydrogen is not exported but hydrogen tanks are. By drawing a service net that includes this information, we have a much better understanding of a system and show the need to use heterofunctional graph theory to analyse a hydrogen system.*

9. Simulation of Hydrocity

The next part of the report is to simulate the events in Hydrocity. The first step to creating a simulation was to make a Petri Net of Hydrocity (Figure 29). The buffers were represented as places, and the transitions between them represent the transportation and transformation processes that occur in the system. After creating the Petri Net, we created production and consumption incidence matrices for each of the operands, relating the places and transitions (Figures 30-35).

For simplicity at this point in the simulation development, all of the weights of the transitions are 1. This could be the case, tracking hydrogen on a mass basis; for example, one kg of gaseous hydrogen should produce approximately 1 kg of liquid hydrogen, if efficiency is high, and could be condensed such that each tank of hydrogen contains 1 kg of compressed hydrogen gas. However, these ratios are likely not representative of reality, and so further research should include investigation of these ratios. Additional further research should include looking into capacities of various buffers.

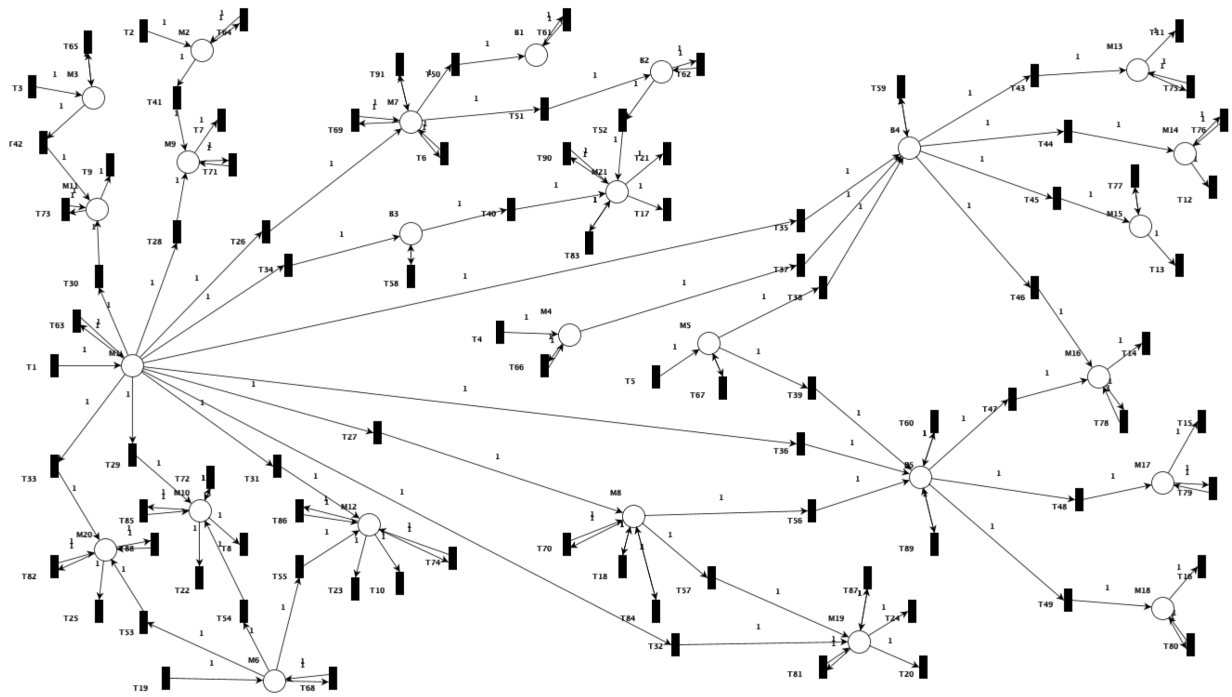

Figure 29 ***Hydrocity Petri Net*** *Based on the sketch and digraph of Hydrocity, we drew a petri net to represent the system to help us analyse and simulate the events in Hydrocity. As we can see, the system is quite complex and has 91 transitions and 26 places. The places are labeled with the same names as assigned for the Network analysis of the system and the transition names correspond to the degrees of freedom they represent (found in Figure 24).*

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
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	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91
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Figure 30 ***Production Incidence Matrix of the Service Net for Gaseous Hydrogen*** *This incidence matrix shows how gaseous hydrogen is created in a place based on the transition. It is a sparse matrix and shows the high degree of freedom in the system.*

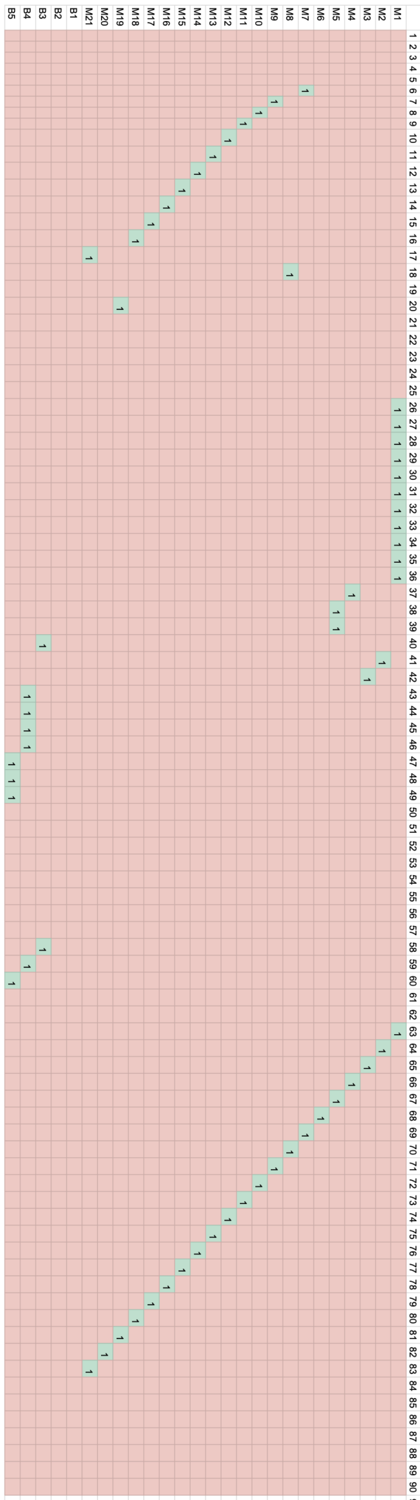

Figure 31 ***Consumption Incidence Matrix of the Service Net for Gaseous Hydrogen*** *The incidence matrix shows how gaseous hydrogen is consumed in a place based on the transition. Once again, this is a very sparse matrix. M1 is the SMR plant and from the consumption incidence matrix alone, it looks like it is the source of hydrogen. Together with the positive incidence matrix of the service net for gaseous hydrogen, they form the gaseous hydrogen incidence matrix for Hydrocity.*

	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	B1	B2	B3	B4	B5
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Figure 32 ***Production Incidence Matrix of the Service Net for Liquid Hydrogen*** *The incidence matrix shows how liquid hydrogen is created in a place based on the transition. As expected from the service net, the production incidence matrix for liquid hydrogen is even sparser than the production incidence matrix for gaseous hydrogen.*

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91
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Figure 33 ***Consumption Incidence Matrix of the Service Net for Liquid Hydrogen*** *The incidence matrix shows how liquid hydrogen is consumed in a place based on the transition. This is a sparse matrix. Together with the*

positive incidence matrix of the service net for liquid hydrogen, they form the liquid hydrogen incidence matrix for Hydrocity.

	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	B1	B2	B3	B4	B5
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Figure 34 ***Production Incidence Matrix of the Service Net for Hydrogen Tanks*** *The incidence matrix shows how hydrogen tanks are created in a place based on the transition. This is a sparse matrix and as expected from the service net, the production incidence matrix is even sparser than the production incidence matrix for gaseous hydrogen.*

	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	B1	B2	B3	B4	B5
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Figure 35 ***Consumption Incidence Matrix of the Service Net for Hydrogen Tanks*** *The incidence matrix shows how hydrogen tanks are consumed in a place based on the transition. Like the production incidence matrix of the service net for hydrogen tanks, the consumption incidence matrix of the service net for hydrogen tanks is also a very spare*

matrix. Together with the positive incidence matrix of the service net for hydrogen tanks, they form the hydrogen tanks incidence matrix for Hydrocity.

After producing all of these incidence matrices, we created a simulation of Hydrocity by following 6 units of hydrogen throughout the system. Using the Petri Net as our guide, we chose 6 viable paths for these units to travel, making sure to represent the production, transportation, storage, and consumption of each operand (Figure 36).

Event Series Description	produce then consume by ammonia plant	import then consume by metal refinery	produce to consume by EV	produce to consume by EV	produce, condense, consume at electricity plant	produce, tank, export
Time	**Firings**	**Firings**	**Firings**	**Firings**	**Firings**	**Firings**
1	1	19	1	4	1	1
2	28	54	36	66	26	63
3	71	22	48	37	6	63
4	71		15	59	51	27
5	7			59	62	70
6				44	62	18
7				12	52	84
8					90	57
9					21	24

Figure 36 ***Events List*** *We imagined how Hydrocity would actually operate in real-life and made a list of events that happen in Hydrocity. We tracked the events at each time step so that we understand what is happening in Hydrocity at each time step. The "Event Series Description" row contains a brief description of the flow of one unit of hydrogen through the system along the transitions listed in the column below each.*

Using the events lists as a guide, we then created the service matrix, which records which transitions are being fired throughout the entire system at any given time step (Figure 37). The final step was to write a MATLAB script, which takes the incidence matrices and the simulation matrices as inputs, and graphically displays the simulation results (see Appendix for script). The script utilizes Definition 4.22 of a Timed Petri Net from [19]. It iteratively (by time step) adds the "existence" of operands to buffers when the transition fired at the given time step has a 1 in the production incidence matrix for the given operand, and subtracts this "existence" of the operand if the transition has a 1 in the consumption matrix for the given operand, resulting in the next state of the system. We recommend running the code with the included attached matrices (included in the Appendix) for the best experience of the simulation. The results of the simulation are shown in Figures 38.

Time Step	1	2	3	4	5	6	7	8	9
T1	4								
T2									
T3									
T4	1								
T5									
T6			1						
T7					1				
T8									
T9									
T10									
T11									
T12							1		
T13									
T14									
T15				1					
T16									
T17									
T18						1			
T19	1								
T20									
T21									1
T22			1						
T23									
T24									1
T25									
T26		1							
T27				1					
T28		1							
T29									
T30									
T31									
T32									
T33									
T34									
T35									
T36		1							
T37			1						
T38									
T39									
T40									
T41									
T42									
T43									
T44						1			
T45									
T46									
T47									
T48			1						
T49									
T50									
T51				1					
T52							1		
T53									
T54		1							
T55									
T56									
T57								1	
T58									
T59				1	1				
T60									
T61									
T62					1	1			
T63		1	1						
T64									
T65									
T66		1							
T67									
T68									
T69									
T70					1				
T71			1	1					
T72									
T73									
T74									
T75									
T76									
T77									
T78									
T79									
T80									
T81									
T82									
T83									
T84							1		
T85									
T86									
T87									
T88									
T89									
T90								1	
T91									

Figure 37 ***Simulation Matrix*** *The simulation matrix shows all of the transitions that are fired at each time step, and how many times they are fired.*

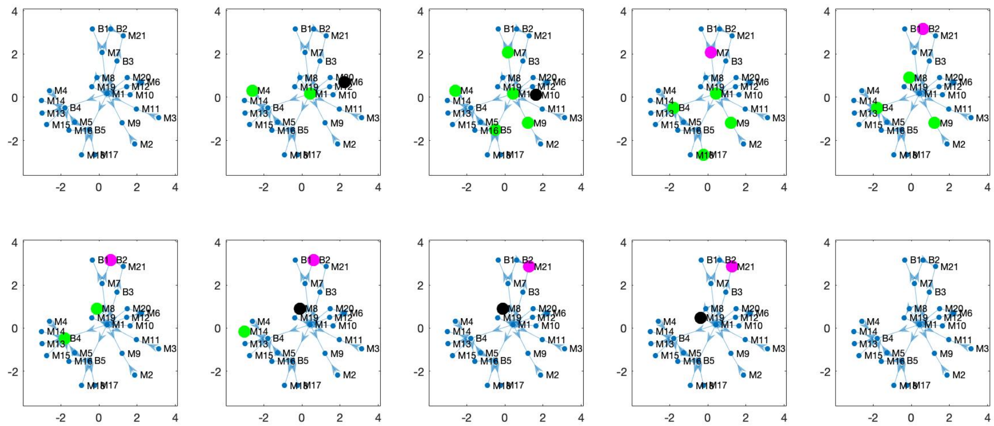

Figure 38 Hydrocity Simulation *These plots show the progressive flow of 6 units of hydrogen through Hydrocity. Green dots represent gaseous hydrogen, pink dots represent liquid hydrogen, and black dots represent tanks of hydrogen. Each plot shows the state of the system at the end of a time step from 0 to 9, starting from the top left and ending at the bottom right. Larger images of each plot are included in the Appendix. Again, we recommend running the attached MATLAB script for the best experience.*

Although the graphical representation is rather crude at this stage, it provides an understandable visualization of the flow of hydrogen through the system. Future steps would include creating a simulation matrix that includes all buffers and transitions, and creating more accurate time steps; combined with more accurate transition weights as well as capacities, the simulation would be an interesting and more accurate representation of the instantiated Hydrocity architecture.

10. Conclusion

As countries around the world transition from a fossil fuel economy towards a hydrogen economy, strategies and policies can be developed through a thorough understanding of the hydrogen economy - what it constitutes and how it performs. The goal of this paper is to offer practitioners, policy-makers and other stakeholders a clear view into the complex network by introducing an invariant reference architecture for the hydrogen economy that not only considers the current state-of-art hydrogen technology, but also realistic potential advancements.

Nevertheless, there may be potential innovations so groundbreaking or too far in the future that it is not considered in this paper; in such case, the reference architecture can be built upon or modified to more accurately reflect the contemporary system. Assuming that this reference architecture remains relevant, the model can serve as a base model for any instantiated architecture of the hydrogen economy, which would further emphasize the parts of the model that are relevant to the specific economy in question.

Both the traditional graph theory and heterofunctional graph theory helps us understand Hydrocity better. However, with heterofunctional graph theory, we are able to understand the system even more as more details are provided to us. From traditional graph theory, we know Hydrocity is a system with many loosely-connected nodes and a central hub. From heterofunctional graph theory, we know Hydrocity is a system with many strongly-connected nodes with a few major central hubs. This shows that Hydrocity is a heterogeneous system with many connections that is not shown with traditional graph theory analysis but with heterofunctional graph theory analysis. This is a good example that shows why heterofunctional graph theory is needed to analyse systems that are very heterogeneous.

Our hope is that the simulation of Hydrocity can provide an example for future research into the optimized development of robust hydrogen economies.

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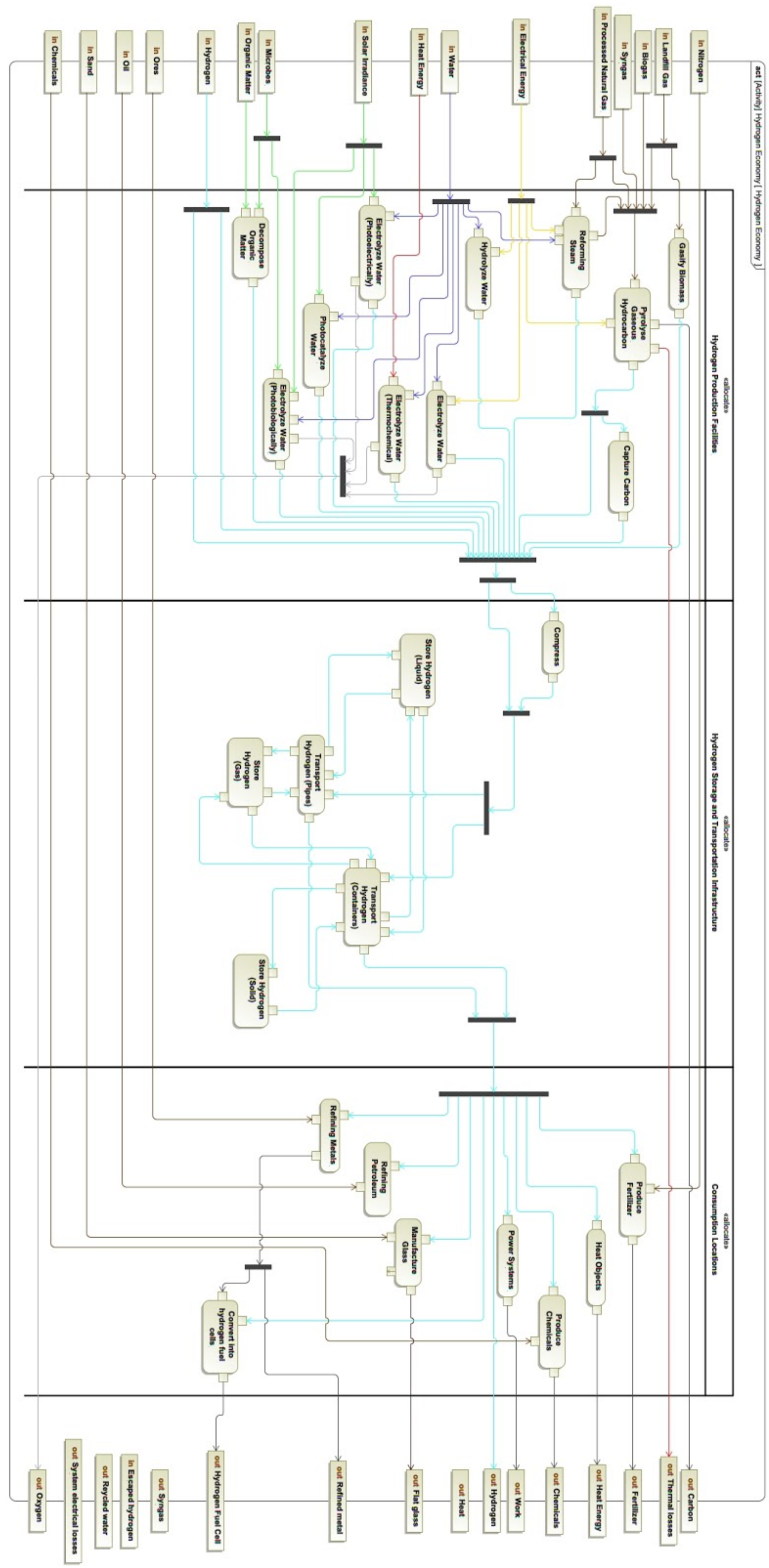
Appendix

Figure A.1 Hydrogen Economy Activity Diagram *The full hydrogen economy activity diagram, separated by lanes.*



MATLAB Script to produce adjacency matrix and associated centrality analyses:

```
% Graphing the adjacency matrix

A = importdata('Formal Adjacency Matrix.xlsx'); %import inflow
 adjacency matrix
N = importdata('Nodes.xlsx');

G_dir = digraph(A);
plot(G_dir, 'Layout', 'force', 'Nodelabel', N);

for x = 1:26
    for y = 1:26
        if A(x,y) == 1 && A(y,x) == 0
            A(y,x) = 1;
        end
    end
end

G = graph(A); % turn into a directed graph

figure
plot(G, 'Layout', 'force', 'Nodelabel', N);
deg = degree(G); % calculate degree node distribution
deg_cent = centrality(G, 'degree'); % calculate in-degree centrality
eig_cent = centrality(G, 'eigenvector'); % calculate eigenvector
 centrality
btwn = centrality(G, 'betweenness'); % calculate betweenness
 centrality
node_dist = 0;
hold = 1;
labels = 0;
for i = 1:max(deg)
    count = 0;
    for k = 1:length(deg)
        if deg(k) == i
            count = count + 1;
        end
    end
    if count ~= 0
        node_dist(hold) = count;
        labels(hold) = i;
        hold = hold + 1;
    end
end

figure
bar(labels, node_dist);
xlabel('node degree');
ylabel('number of nodes');
title('Node Degree Distribution');

% deg_cent
% eig_cent
```

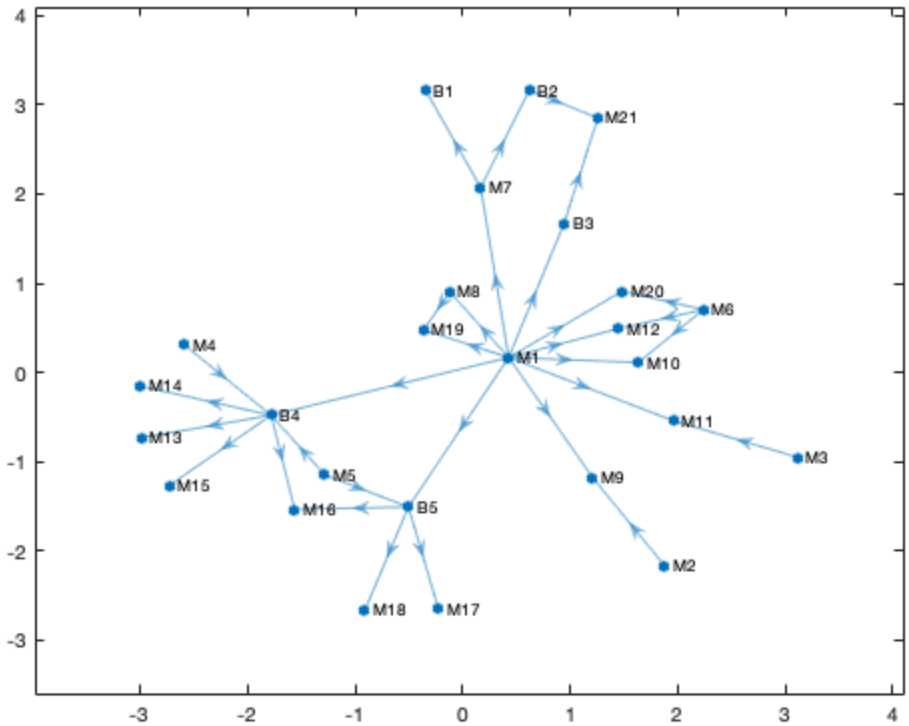
```
% btwn

T = table(N, deg_cent, eig_cent, btwn)
%T.Properties.RowNames = N;
% col = {'Node', 'Degree Centrality', 'Eigenvector Centrality',
 'Betweenness Centrality'};
% T.Properties.RowNames = N;
% figure
% plot(T{:,:})
%uitable('Data',T{:,:},'ColumnName',col, ...
   % 'RowName', N, 'Units', 'Normalized', 'Position',[0, 0, 1, 1])
```

T =

26×4 table

N	*deg_cent*	*eig_cent*	*btwn*
'M1'	11	0.14581	244.5
'M2'	1	0.010602	0
'M3'	1	0.010602	0
'M4'	1	0.020632	0
'M5'	2	0.038029	5
'M6'	3	0.037217	1.5
'M7'	3	0.045088	45
'M8'	2	0.051322	0
'M9'	2	0.040721	24
'M10'	2	0.04765	7.3333
'M11'	2	0.040721	24
'M12'	2	0.04765	7.3333
'M13'	1	0.020632	0
'M14'	1	0.020632	0
'M15'	1	0.020632	0
'M16'	2	0.038029	5
'M17'	1	0.017397	0
'M18'	1	0.017397	0
'M19'	2	0.051322	0
'M20'	2	0.04765	7.3333
'M21'	2	0.014968	1
'B1'	1	0.011738	0
'B2'	2	0.015635	2
'B3'	2	0.041858	21
'B4'	7	0.079248	106.5
'B5'	5	0.06682	63.5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B5
M2
M18
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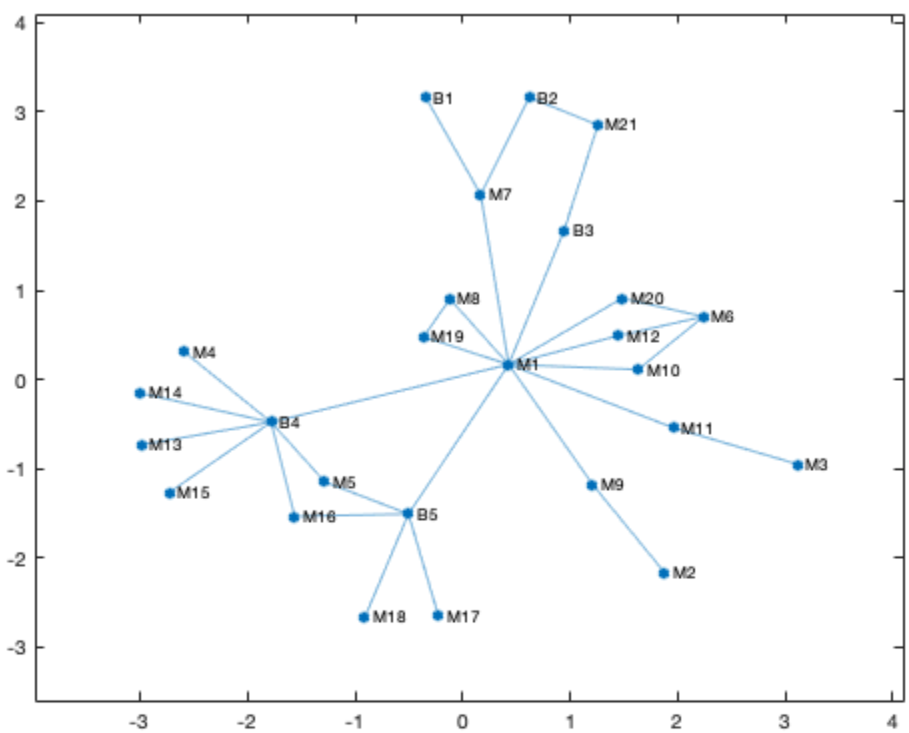
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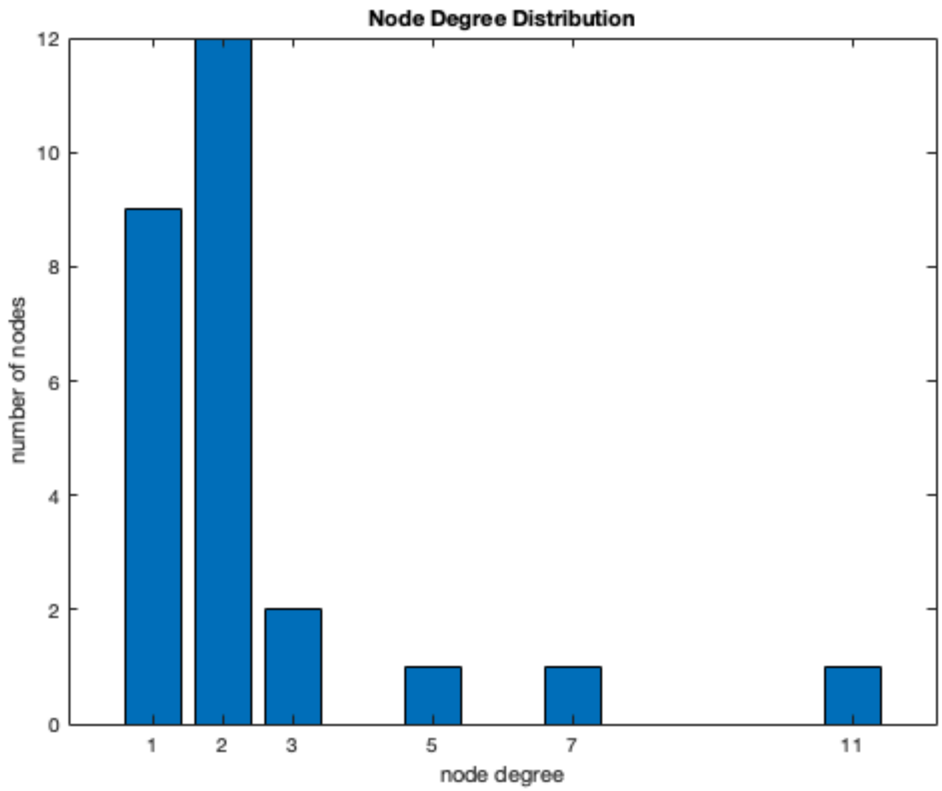
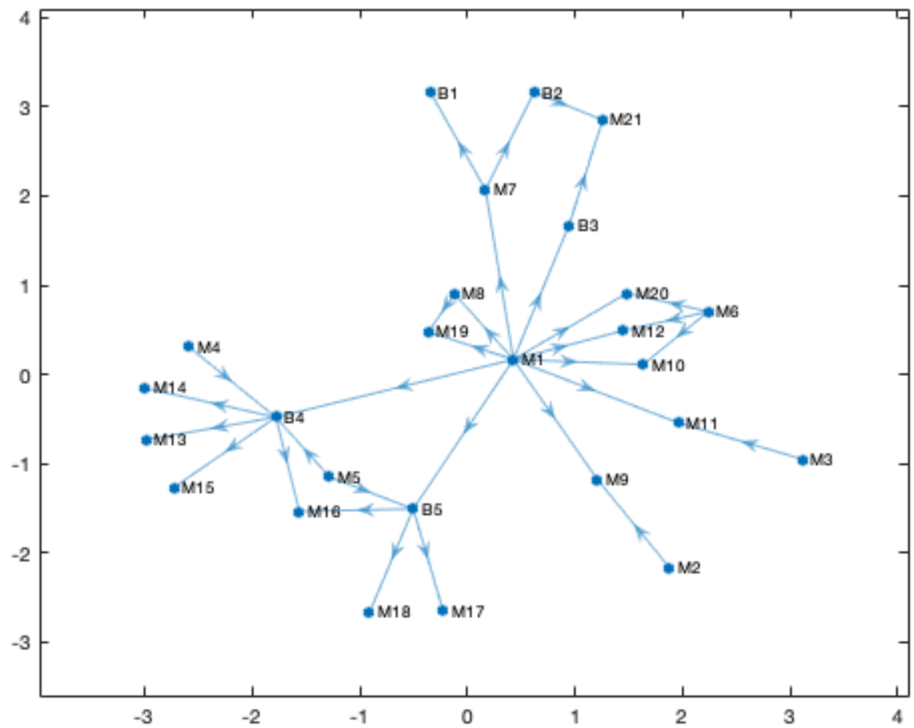


Published with MATLAB® R2018a

MATLAB Script used to produce Simulation:

```
% Emma Doherty
% ENGS 199 - 21W

% Hydrocity Simulation

% Incidence matrices: each 26 buffers x 91 DOFs:
Mp_gas = importdata('gas prod.xlsx'); % gas production
Mc_gas = importdata('gas con.xlsx'); % gas consumption
Mp_liq = importdata('liq prod.xlsx'); % liquid production
Mc_liq = importdata('liq con.xlsx'); % liquid consumption
Mp_tank = importdata('tank prod.xlsx'); % tank production
Mc_tank = importdata('tank con.xlsx'); % tank consumption

A = importdata('Formal Adjacency Matrix.xlsx'); %import inflow
 adjacency matrix
N = importdata('Nodes.xlsx'); % import node labels

initial = zeros(26,1); % state of system (each buffer) at time t = 0

simulation = importdata('simulation 1.xlsx'); % DOF (91) x #events

[r,c] = size(simulation);
events = c; % number of time steps in simulation

% matrices to describe flow of operands through buffers:
state_gas = [initial, zeros(26, events)];
state_liq = [initial, zeros(26, events)];
state_tank = [initial, zeros(26, events)];

% gaseous hydrogen:
for count = 1:events
    state_gas(:, count+1) = state_gas(:, count) + Mp_gas*simulation(:,
 count) - Mc_gas*simulation(:, count);
end

% liquid hydrogen:
for count = 1:events
    state_liq(:, count+1) = state_liq(:, count) + Mp_liq*simulation(:,
 count) - Mc_liq*simulation(:, count) ;
end

% tank hydrogen:
for count = 1:events
    state_tank(:, count+1) = state_tank(:, count) +
 Mp_tank*simulation(:, count) - Mc_tank*simulation(:, count) ;
end


G_dir = digraph(A); % create directed graph of system

for count = 1:events+1
    % plot the state of the system at the end of each time step:
```

```
    n = 1;
    m = 1;
    p = 1;
    h_gas = 0;
    h_liq = 0;
    h_tank = 0;

    % determine which nodes to highlight for each operand at each time
    % step, and store these in vectors:

    for i = 1:length(state_gas)
        if state_gas(i, count) ~= 0
            h_gas(n) = i;
            n = n+1;
        end
        if state_liq(i, count) ~= 0
            h_liq(m) = i;
            m = m+1;
        end
        if state_tank(i, count) ~= 0
            h_tank(p) = i;
            p = p+1;
        end
    end

    % plot state of system at the end of this time step:
    figure
    p1 = plot(G_dir, 'Layout', 'force', 'Nodelabel', N);

    if h_gas ~= 0
        highlight(p1, h_gas, 'NodeColor', 'g', 'MarkerSize', 10);
    end

    if h_liq ~= 0
        highlight(p1, h_liq, 'NodeColor', 'm', 'MarkerSize', 10);
    end
    if h_tank ~= 0
        highlight(p1, h_tank, 'NodeColor', 'k', 'MarkerSize', 10);
    end

    pause(2)

    % clear variables:
    clear h_gas;
    clear h_liq;
    clear h_tank;
    clear a;
    clear b;
end
```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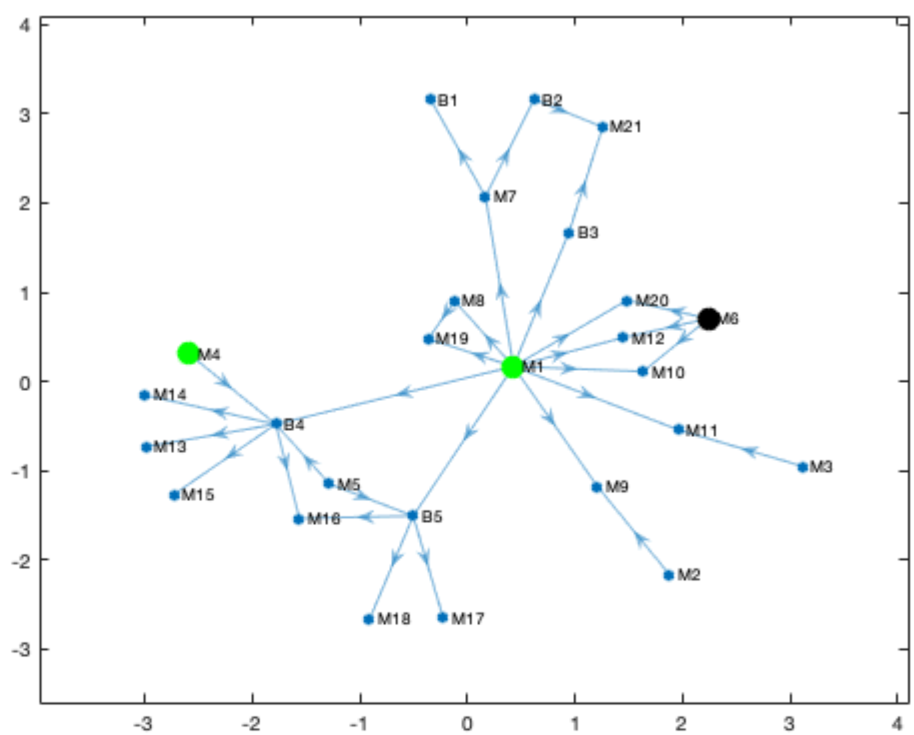
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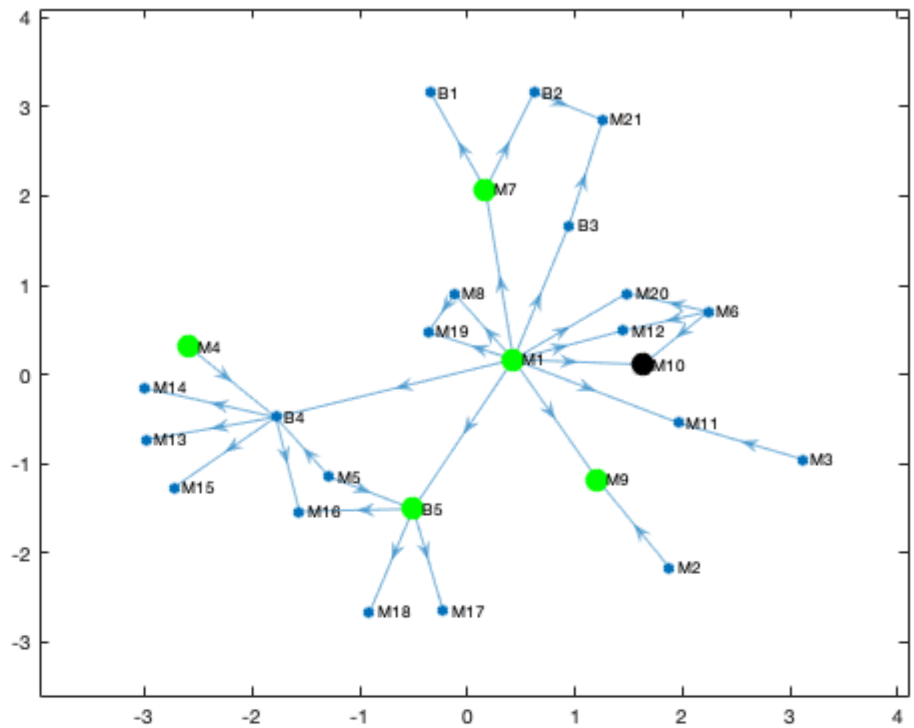
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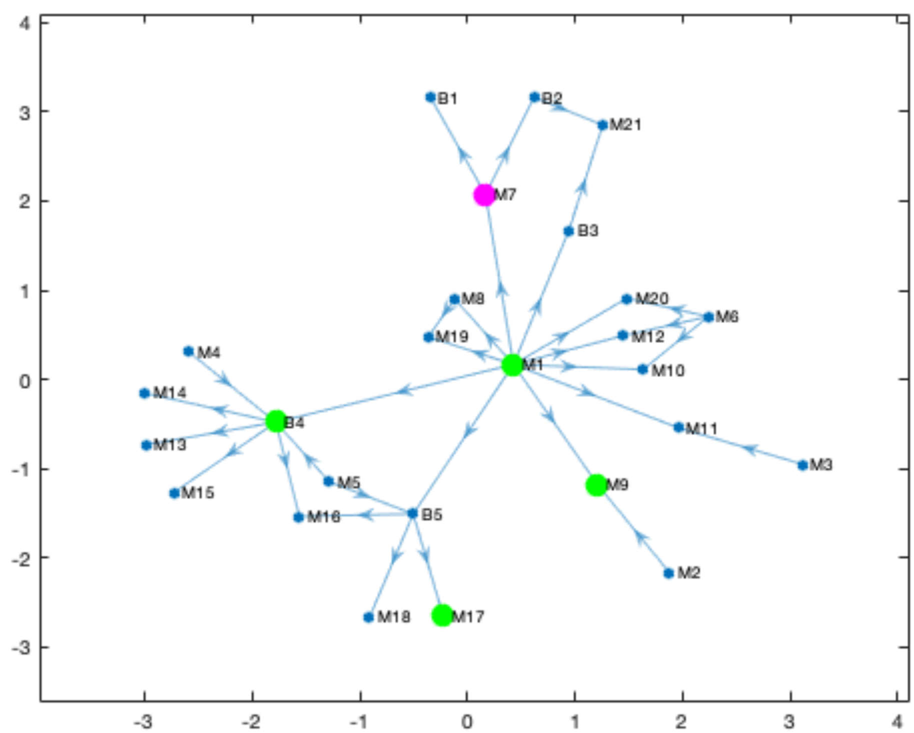
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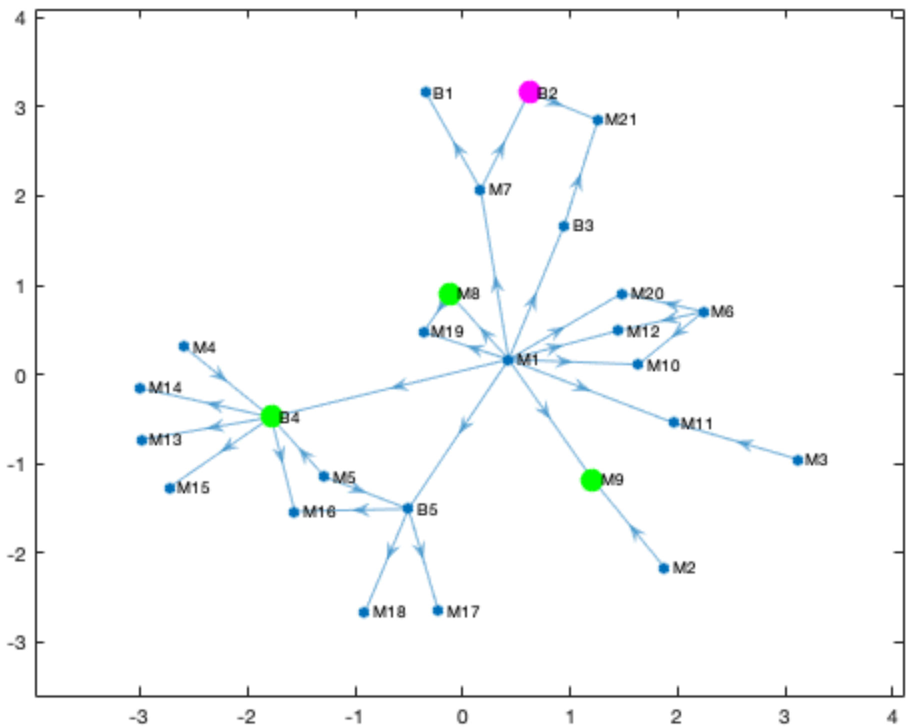
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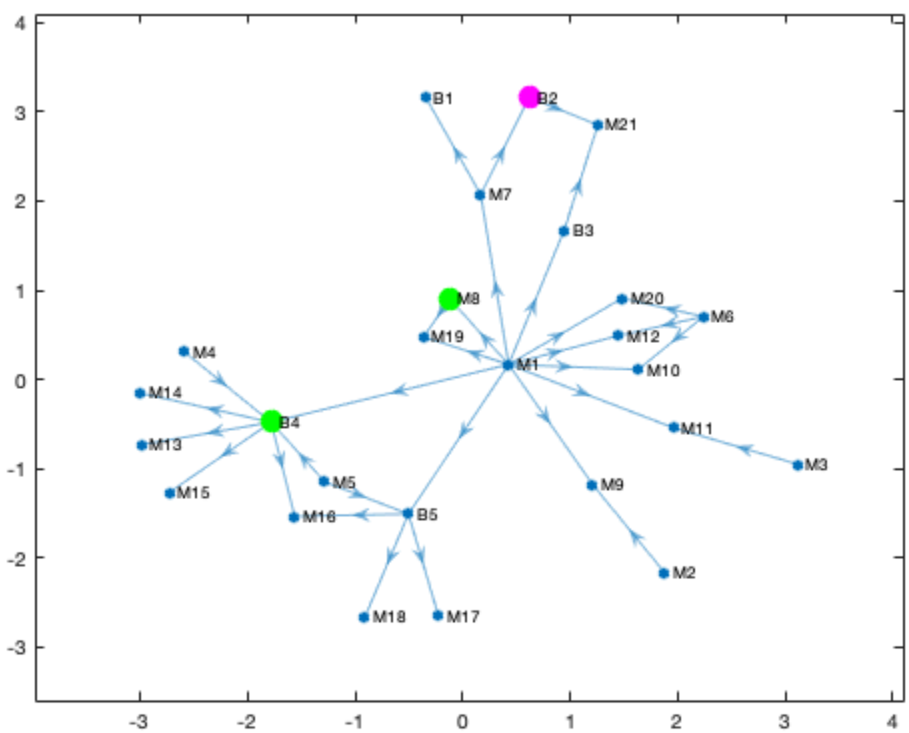
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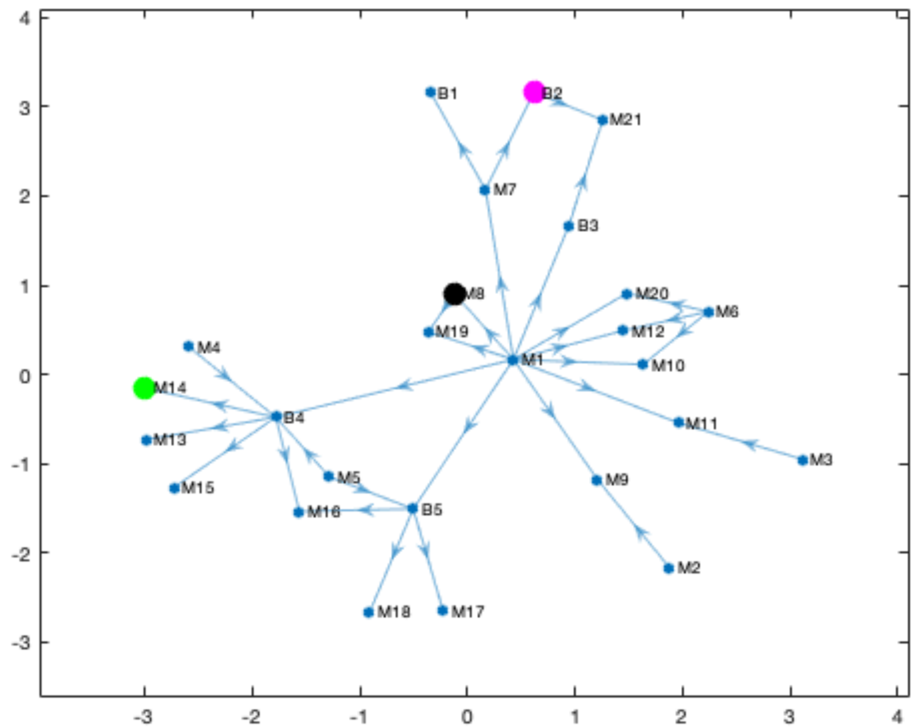

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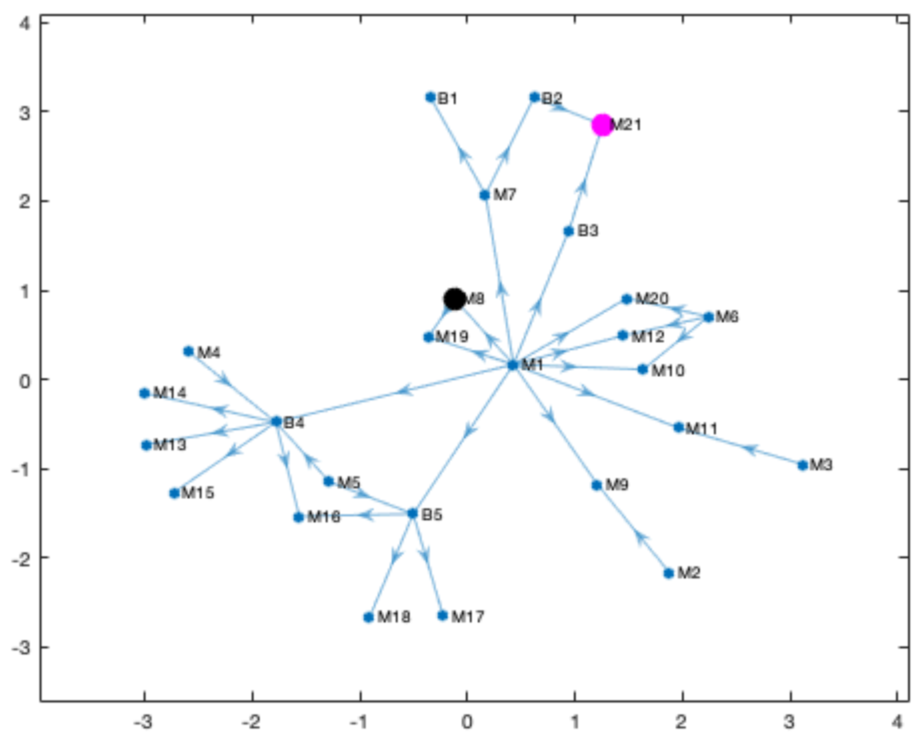

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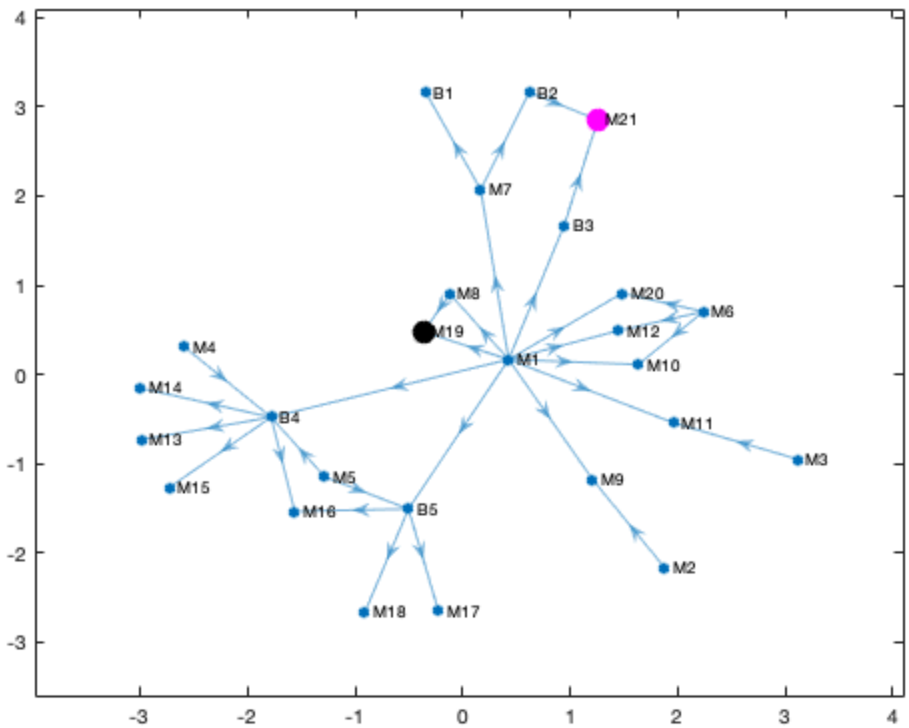
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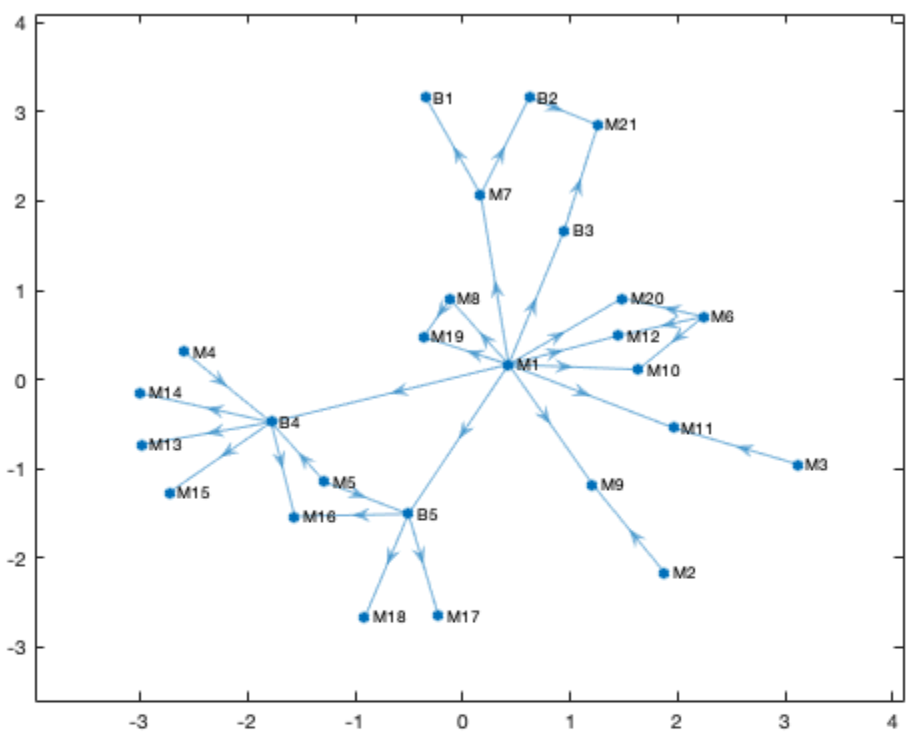
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