

Sustainable Fuel Aviation Infrastructure and Transition: Hybrid Agent-Based Modeling and System Dynamics

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Abstract — The adoption of sustainable fuels in aviation, such as Sustainable Aviation Fuels (SAF), hydrogen (LH2), and ammonia (NH3), is a significant step toward achieving green and sustainable air transport. However, transitioning the aviation industry to sustainability is a complex process that requires an integrated transformation of both technological and social systems. With multiple potential fuel alternatives, it is important to identify the most viable fuel pathways. This paper presents the concept of a hybrid, Agent-Based Modeling (ABM) and modular System Dynamics (SD) model, developed as a computational framework to analyze the interactions among technology, industry, markets, and society. A hybrid ABM and SD approach is an ideal choice for analyzing the transition of the ATS to sustainable fuels because of the complexity of the problem, which involves various entities with distinct behaviors and decision-making processes. The modular SD model consists of multiple stock and flow modules of passenger demand, aircraft orders, fleet development, fuel demand, sustainable fuel production, and infrastructure, providing a holistic but detailed, granular analysis of interactions and impacts within the system. The ABM approach facilitates the integration of SD modules by incorporating agents such as airlines, fuel suppliers, airports, aircraft manufacturers, and fuel producers, each with their unique behaviors. The proposed model serves as a reference framework for simulation and analysis, supporting future research on aviation sustainability and providing a decision-support tool for understanding the long-term feasibility of different sustainable aviation fuels.

Keywords—Agent-Based Modeling (ABM), Causal Loop Diagram (CLD), hybrid modeling, System Dynamics (SD), Sustainable Aviation Fuels (SAF), aviation energy transition, simulation

I. INTRODUCTION

Responsible for about 2-3% of global energy-related CO₂ emissions, aviation is considered to be the most polluting mode of transport in terms of emissions emitted per passenger kilometers [1], [2]. Amid escalating global concerns regarding climate change, the aviation industry faces an unprecedented challenge to decarbonize and reduce its environmental impacts. The industry has set itself a target to achieve climate neutrality by the year 2050 [3]. To achieve this, several key focus areas have been identified and amongst which energy infrastructure is a key focus area that covers both fuel (energy) technologies and the necessary infrastructure for their adoption. In particular, it encompasses a transition of the Air Transportation System (ATS) from kerosene-based fuel to more sustainable fuel options, such as Sustainable Aviation Fuel (SAF), Liquid Hydrogen (LH2), and Ammonia (NH3)

amongst other options as a replacement of kerosene-based fuels. It also includes infrastructure needed to support this transition [1].

However, the ATS is an inherently complex sociotechnical system that involves multiple stakeholders and consists of a number of technical and non-technical elements and interdependencies to deliver effective system capabilities and goals. Furthermore, it is also very dynamic, implying, any change in the system elements will have a significant impact on other system elements and the system as a whole. These characteristics make the transformation of the ATS a complex process requiring an integrated transformation of both technological and social systems. Therefore, understanding the multifaceted transition of the ATS to sustainability, as characterized by these complex sociotechnical interactions and dynamic behaviors, necessitates adoption of methodologies that can effectively capture interdependencies and their impacts on the overall system performance.

In this context, simulation-based methods are considered as powerful tools to evaluate and analyze complex sociotechnical systems. Among various simulation-based methods, Agent-Based Modeling (ABM) and System Dynamics (SD), are widely used for analyzing complex systems [4]. These approaches can be applied as standalone methodologies to evaluate and optimize system performance. However, at times, a single approach is not sufficient to model complex systems, and in such scenarios two or more methodologies can be combined to develop a hybrid simulation model [5]. This allows the methodological limitations of any single method to be overcome and better representation of system elements and their behavior.

This paper presents the concept of a hybrid ABM and modular-SD simulation model of the ATS as a computational framework to analyze the interactions among technology, industry, markets, and society. ABM is a natural choice for analyzing the transition of the ATS to sustainable fuels because of the complexity of the problem. The ATS transition to sustainability problem involves a variety of entities, each with its own behavior and decision-making process, and can be effectively represented as agents. For example, a fuel supplier can be modeled as an agent that informs its behavior in terms of production and pricing in response to market dynamics. On the other hand, SD is a particularly relevant methodology for studying and managing complex ATS subsystems, especially those characterized by feedback loops, time delays, and stock accumulations [6]. SD aims to describe

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system evolution over time by showing information feedback in the system. It involves a qualitative approach (causal loop diagram) and a quantitative approach (stock and flow and simulation models) to develop robust information feedback structures through simulation or optimization [7]. Many authors have employed SD modeling and simulation in diverse domains to examine and explain the general principles underlying sociotechnical system dynamics over time [8].

Hybrid simulation models combining ABM and SD are increasingly being utilized to analyze complex systems [9], [10]. For instance, in the automotive sector, [9] developed a hybrid framework to support manufacturers' product strategy decisions for alternative fuel vehicles. In their model, ABM was used to simulate individual customer agents making purchase decisions and SD captured the broader market dynamics. Similarly, in the field of urban planning, [10] applied a hybrid ABM-SD model to evaluate policies aimed at reducing CO₂ emissions from transportation in Beijing.

In the specific context of the ATS transition to sustainable fuels, current research primarily focuses on the drivers and barriers to the adoption of sustainable fuels. For example, the study by [11] investigated obstacles to sustainable biofuel transition from a sociotechnical standpoint, using a multi-level perspective SD model. The authors propose policies and strategies to affect the transition. Similarly, [12] studied the drivers and barriers in the adoption and diffusion of sustainable jet fuel, highlighting the critical role of airlines and jet fuel buyers as the main drivers. Authors reported that main barriers to adoption include government policies, high production costs, fuel logistics, and quality control issues during blending, transportation, and storage. However, these studies are limited in scope due to their focus on a specific fuel technology, predominantly SAF. Considering that multiple competing alternatives exist, including LH₂, NH₃, and SAF among others [1], [13], it becomes crucial to shed light and understand which sustainable fuel option would likely shape the future pathway. Furthermore, these previous studies did not consider disruptions and potential strategies to mitigate their impact by building ATS resilience. Therefore, this study aims to address the gaps highlighted above. To do so, a hybrid ABM and SD simulation model is developed to analyze the transition of ATS to sustainable fuels. The developed model study specifically aims to address two key questions: (1) *Which fuel technology is likely to become ready first*, and (2) *How do disruptions in passenger demand and fuel supply affect various aspects of system performance across different scenarios*.

This study adopts the modular SD approach used by Thies [14] in the simulation of sustainable fuel supply chains in aviation and integrates it with an agent-based approach. While the study by [14] focused on SD modeling of alternative fuel supply chains, particularly fuel production capacity, this study presented in this paper expands the scope by incorporating fuel infrastructure development, including storage and distribution. Furthermore, this study integrates the modular SD framework with ABM and introduces decision-making agents, such as airlines, fuel suppliers, and aircraft manufacturer. Adopting the hybrid approach allows for a more realistic representation of the sociotechnical elements within the ATS, their interactions and decision-making processes. Each agent operates its own SD module that governs its behavior, interactions and responses within the broader system. An agent-based representation is crucial for

incorporating decision making capabilities into the model, enabling the observation of how individual decisions impact the broader system. This approach facilitates understanding of long-term fuel adoption pathways, enabling stakeholders to assess how different factors—such as infrastructure readiness, fleet transitions, and policy incentives—interact over time. The model enables understanding of key variables that influence and accelerate the transition of the ATS towards sustainable fuels, both at the agent and the whole system level. The output of this study is expected to provide insights for industry and policymakers.

The contributions of the study are summarized as follows:

1. A conceptual model developed as a part of the study is presented, integrating the ABM and modular SD framework.
2. A modular Causal Loop Diagram (CLD) and an example of a SD module detailing stock and flow diagram is provided to identify the feedback structure in the system; and
3. The transition from modular SD into hybrid ABM-SD is presented and illustrated via an example case.

The paper is organized as follows. Section II provides an overview of the methodology adopted. In Section III, the agent-based and modular SD conceptual framework are presented and system architecture where individual SD modules are discussed. Next, Section IV describes the modular CLD developed to illustrate how variables influence each other creating a feedback mechanism. Subsequently, Section V discusses and demonstrates the approach adopted for the conversion of an SD module to an active decision-making agent. Finally, the conclusion is provided in Section VI.

II. METHODOLOGY

This study presents the concept of a hybrid agent-based and modular SD model. This is a holistic framework to analyze the interactions and interdependencies among sociotechnical factors.

A. Agent Based Modeling.

ABM is a computational method used to simulate the interaction between different system components or entities to study the overall system behavior as it emerges from such interactions [15]. System components are modeled as individual agents that have their own states and behaviors. ABM is adopted in this study for four key reasons. First, ABM enables a bottom-up modeling approach, starting with individual agents and the system behavior emerges from agent interactions. This approach conforms with the context in which individual components including airport, and aircraft manufacturer, can be modeled individually while the emergent system behavior cannot be inferred using a top-down approach. Second, ABM supports heterogeneity, where agents with diverse behaviors and characteristics can be modeled, unlike other modeling approaches that are difficult with heterogeneous components, such as equation-based modeling. Third, ABM is highly flexible, allowing the modeling of each entity and its complex behavior independent of other components. This is lacking in other modeling approaches including SD, where the focus is on representing component behaviors in a variable flow form. Finally, ABM supports decision making and adaptive agent behavior, where the agent can learn from its interactions. This is important to capture the changing dynamic behavior of components such as airlines, society, and fuel suppliers [16].

B. Modular System Dynamics Modeling

A modular structure allows for comprehensive and granular analysis of key components of SD modules, which consist of stock and flow models, while maintaining a comprehensive system-wide perspective. The modular approach for SD models also provides flexibility and scalability allowing the representation of systems with varying levels of complexity and size. In this study, the SD modules include passenger demand, aircraft orders, fleet development, fuel demand, fuel infrastructure (including storage and distribution) and sustainable fuel production.

The SD modeling process consists of qualitative SD models which involve knowledge elicitation and presentation to explain the structure and behavior of the system, and quantitative SD models which involve computer simulations to predict system behavior. A key qualitative approach within SD modeling is the use of the CLDs that consist of a series of variables (or factors) and arrows that link these variables to reveal the dynamic interconnected nature of a system by showing the causal relationships and feedback in a system [17]. A modular CLD is developed to provide a comprehensive view of the entire system by illustrating the relationships of different variables including variables of one module and the other modules.

The quantitative SD describes the system in terms of stocks (also called levels), flows (or rates) and converters (or auxiliary variables) that represent the dynamic of the system. A stock and flow diagram which is commonly derived from a CLD presents the relationship of stocks, the accumulated quantities within the system, and flows, which represent changes to the stocks that occur during a period of time. A simulation process to study the evolution of the system overtime can be conducted by entering the initial value and equation for stock such as the population size considered within the Passenger Demand module and parameter values and equations for other variables such as population growth rate, Gross Domestic Product (GDP) and GDP growth rate. The information for the values and behavioral relationship to be entered in a simulation model can come from any available sources such as observations, interviews, company records, historical records and statistical analysis [17], [18]. In this study, the stock and flow diagrams are developed for each SD model to facilitate a detailed analysis of each module. These individual diagrams and simulation components are then integrated into a comprehensive system simulation with a detailed and interconnected view of the overall system dynamics.

C. Integration of ABM

The model incorporates decision-making capabilities within agents, which were previously modeled as passive entities. While the internal dynamics of these agents continue to be represented through SD simulation, they now include decision-making ability. This approach follows the approach outlined in [19] and the steps involved are as follows. First, variables, stocks, and flows are identified, and the agents that could represent these variables are determined. Second, model equations are used to specify agent behavior. Third, flows and feedback loops are used to identify agent interactions. Finally, the initial conditions defined in the model are used to initialize the state of each agent.

III. SYSTEM ARCHITECTURE AND CONCEPTUAL MODEL

A high-level system architecture illustrating different sociotechnical elements included in this study is presented in Fig. 1. The architecture serves as a blueprint depicting key agents, SD modules, and interactions, which constitute the model and their interrelationships. The agents have their internal behavior modeled with SD modules, with stock and flows. The agents interact with each other and will include decision making capability. Modules are modeled as active agents which interact with each other and make decisions. Each SD module and its related agent are detailed in this section.

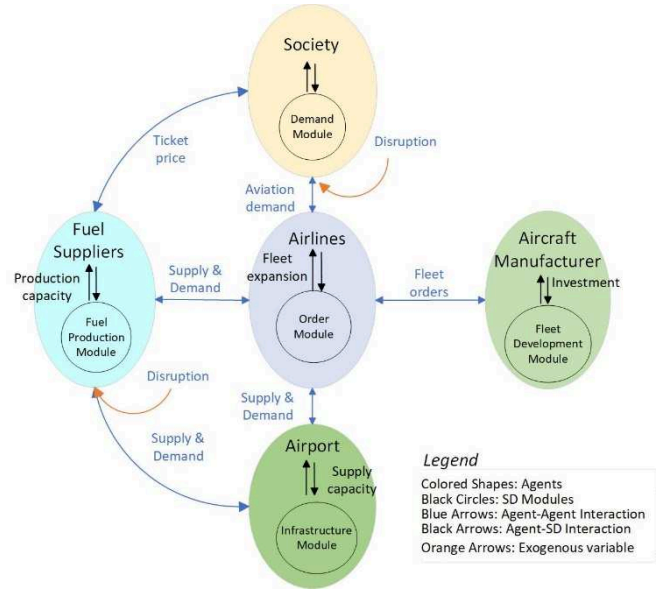


Fig. 1. Overview of the agent-based and modular system dynamics conceptual framework.

A. Society Agent: Passenger Demand and Flight Demand Modules

At the top of Fig. 1, within the *Society* agent, lies the Passenger Demand module. The module's purpose is to model and simulate passenger demand for different categories of flights including short distance, medium distance, and long distance. It also covers passenger behavioral aspects reflecting preferences for green or sustainable aviation. Furthermore, as depicted in Fig. 1, the module considers potential disruptions in passenger demand as an exogenous variable. This module translates passenger demand into Revenue Passenger Kilometers (RPKs), a standard metric used in the aviation sector. The output of the module is expected to inform the *Airlines* agent about the expected demand for each flight category.

B. Airlines Agent: Order Module

Aviation passenger demand, emanating from the *Society* agent's Demand module directly feeds into the Flight Demand Order module within the *Airlines* agent. This module is considered to be a passive agent in the simulation model that translates passenger demand into revenue passenger kilometers. The output of the order module is expected to inform the *Airlines* agent about the expected demand for each flight category. The module determines the stock of

operational flights and subsequently computes the airlines' carrying capacity, measured in available seat kilometers (ASKs), segmented by flight class. The module then estimates the stock of existing operational flights and computes the airline's carrying capacity in ASK, for each flight class. ASKs are then compared against the demand (RPKs) to calculate the demand-capacity imbalance, which is then used to generate orders for new aircrafts. These orders are sent to the *Aircraft Manufacturer* agent (located to the right of the *Airline* agent in Fig. 1) and provide input to the fleet development module.

Another function that the *Airline* agent performs is to dynamically account for ageing aircrafts by tracking their service life and remaining operational life. This is used to identify and retire ageing aircrafts from the pool of operational aircrafts as they reach the end of their lifecycle. Furthermore, the module interacts with the Infrastructure and the Fuel Production modules within the *Airport* and *Fuel Supplier* agents, respectively. Fuel demand estimates are obtained by considering the number and the types of aircraft, their respective average fuel consumption rate and average flight distance.

C. Aircraft Manufacturer Agent: Fleet Development Module

This module is responsible for manufacturing different types of aircrafts as ordered by the *Airlines* agents. The *Manufacturer* agent represents the aircraft manufacturing sector which responds to airline orders by delivering aircraft of different types. Once an order is received, a new aircraft manufacturer process is initiated, after which the aircraft is delivered to the airlines to become a part of its fleet.

D. Airport Agent: Infrastructure Module

Fuel infrastructure is a critical aspect for ATS functionality. In the context of this study, it refers primarily to storage and distribution. For the adoption of any new technology, for example LH2, infrastructure needs storage and transportation facilities and sufficient capacity which necessitates investments. These variables and their interrelationships are considered in this module which are modeled using stocks and flows.

E. Fuel Supplier Agent: Fuel Production Module

The Fuel Production module models the production of fuels using available feedstock, technology and capacity. The produced fuel is then supplied to aircraft via supply infrastructure. The module receives information about the expected demand for different types of fuels from the *Airlines* agent. It also interacts with the *Airport* agent about the supply and storage infrastructure capacity.

It is to be noted that in Fig. 1, a generic representation of single Infrastructure and single Fuel Production modules are shown, however, in the actual model, multiple modules (or agents) exist, each corresponding to a specific fuel technology and infrastructure, including LH2, ammonia and SAF in this instance. For illustration purposes, an example of the LH2 production module is discussed in the next section. Moving further, the fuel from the producers is supplied via infrastructure which has its own capacity constraints.

IV. MODULAR CAUSAL LOOP DIAGRAM (CLD)

To understand the complex nature of the system, Fig. 2 shows a CLD, showing different modules (color-coded) introduced in Fig. 1, which are interconnected with each other and interrelated in a semantic way. The interrelationships of sociotechnical factors associated with passenger and flight demand, airlines, fleet development, infrastructure, and fuel production are illustrated in the CLD.

The variables on the top-left of Fig. 2 (orange) represent the feedback and interrelations within the Demand module. It can be observed from the CLD that the total demand variable (for air travel) is influenced by external factors such as GDP, public awareness for sustainable flights, and population, as well as internal factors such as average ticket price, price elasticity of demand, and system congestion [20], [21]. Consequently, total aviation demand for sustainable air transport is modeled as a function of per capita GDP, which shows how population can afford a specific transport system, and several other factors, such as flight fare, public awareness for sustainable transport, and capability of airlines to provide the service without congestion.

The next relationship that the CLD in teal green depicts corresponds to the total flight demand. This variable is linked

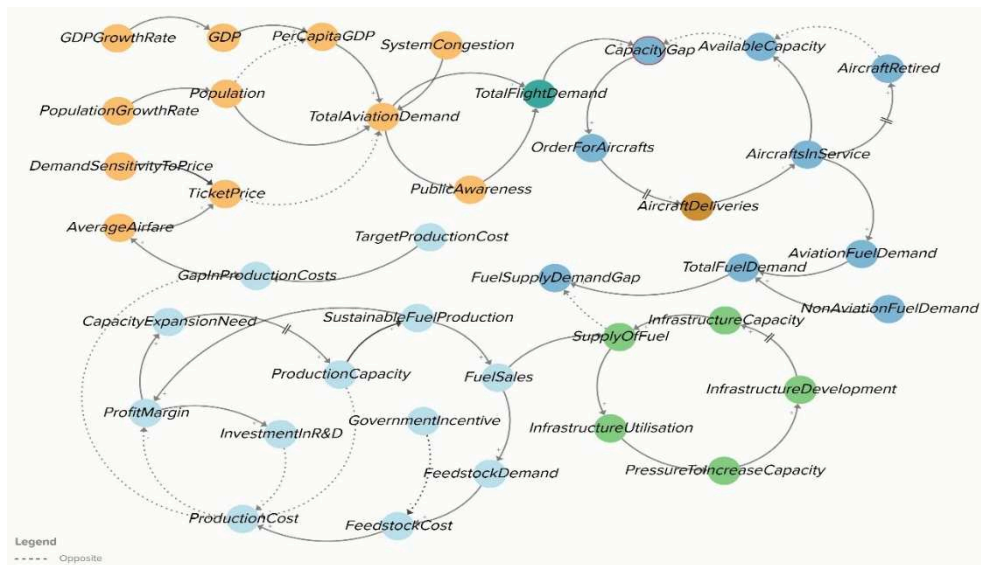


Fig 2. The causal loop feedback diagram showing different modules and their dependencies and interrelationships in a color-coded format.

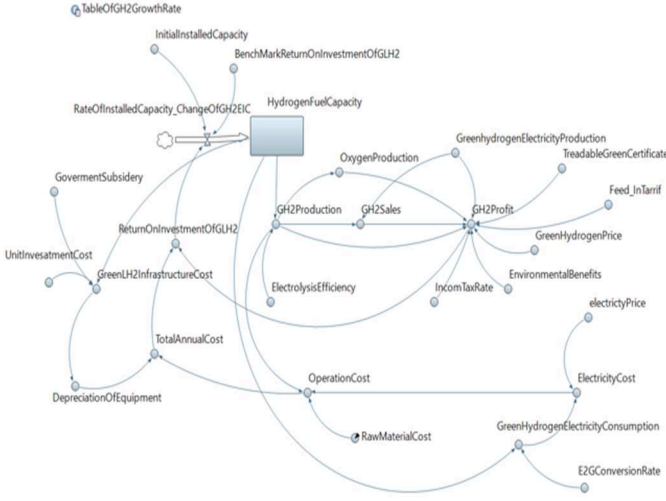


Fig. 3. Stock and flow model of the LH2 production.

with the total aviation demand and the passenger awareness factor, representing passengers' preference for sustainable options. The variable is modeled as an array and consists of demand or three aircraft types, categorized according to flight distance. Moving ahead, the CLD now shows that the total flight demand variable then feeds to the *CapacityGap* dynamic variable. This variable is a function of available capacity, measured in terms of available seats kilometers (ASKs), and demand in terms of RPKs; moreover, it informs the available capacity depends on the total number of operational aircrafts, which is also used in estimating fuel demand. Gap in fuel demand is computed by considering the demand for fuel and the minimum of supply infrastructure capacity or the production capacity. Supply infrastructure CLD is shown in green. The CLD reveals that as the fuel demand increases the requirement of fuel increases. This leads to an increase in the supply and the utilization of the infrastructure. As utilization level increases to a sufficiently high value, the need for capacity expansion also goes up. This triggers capacity expansion activity and after a time delay more storage and distribution capacity is added to the infrastructure.

Similarly, for the fuel producers, the CLD highlights that the fuel supply depends on the production capacity and demand. As more fuel is sold, producers start to make more profits which would lead to more money invested in the research and development of fuel technology that again would lead to a reduction in the production costs. Moreover, production capacity itself is dependent on the profit margins.

As the sale of the fuel increases, the cost of production comes down due to the economies of scale coming into play. As the cost of production falls, profit margins go up; as a result, the producers have more incentive to invest in the capacity expansion. Furthermore, as the production costs go down, ticket prices move in the same direction which leads to an increase in demand and creates a reinforcing loop.

The CLD in light blue on the bottom left corner illustrate the feedback mechanisms governing sustainable fuel production within the air transportation system. For fuel producers, the CLD reveals that fuel supply is a function of both production capacity and demand. Increased fuel sales generate higher profits, incentivizing investment in research and development (R&D). This R&D investment, in turn,

drives down production costs, further boosting profit margins and creating a reinforcing feedback loop. Furthermore, production capacity itself is influenced by profit margins. As fuel sales rise, economies of scale come into play, leading to reduced production costs. These lower costs increase profit margins, providing producers with greater incentive to invest in capacity expansion. This expansion increases fuel supply, which can, in turn, lower prices and stimulate further demand. The lower production costs also have a direct impact on ticket prices. As fuel costs decrease, airlines can offer lower fares, leading to increased demand and completing another reinforcing loop.

V. Agent-Based Model

As an illustration, this paper focuses on the *Fuel Supplier* agent and Fuel Production module, specifically on the *LH2 Supplier* agent. Below is a screenshot of the Green Hydrogen (GH2) production SD module, produced through electrolysis using renewable energy before it is liquified, developed using AnyLogic simulation software (Fig. 3). The core stock variable identified in this context is the production capacity of GH2. As can be seen from the figure, the production capacity is dynamically influenced by factors such as installed capacity, initial capacity levels, electrolysis efficiency, and the profitability of hydrogen production. Profitability, in turn, is affected by hydrogen and power sales revenues, which depends upon infrastructure and operational costs, government subsidies, and market mechanisms like Tradable Green Certificates and power market prices. Next, equations governing the behavior of the agent were specified. These equations are not explicitly listed here, but govern the calculations of capacity, profits and so on. The figure shows key feedback loops and depicts that, for example, the production cost of GH2 is expected to decrease annually, as the production efficiency increases due to technological progress, also known as the learning rate. Furthermore, it could be observed that the government policy plays a critical role in controlling the electricity costs for hydrogen production via subsidies on infrastructure investments and income tax rates.

Algorithm: Pseudocode for LH2 production growth rate expansion decision.

```

1  Input parameters: target_profit_margin,
   growth_rate_change
2  while true:
3      // Observations from the system.
      Current profit margin, return_on_investment
      Current demand, current_demand
      Current production capacity,
      current_production_capacity
4      if return_on_investment >= target_profit_margin
5          if current_production_capacity < current_demand
6              production_growth_rate =
              growth_rate_change
7          else
8              do nothing
9      else
10         current_production_capacity -=
            growth_rate_change
11         Update production capacity growth rate in the SD
           module

```

Note: words in *italics* represent variables in the model

Fig. 4. Proposed algorithm.

To incorporate decision-making capabilities, several key agent decisions are identified, one of which is the control of production capacity growth rate for LH2 production. Although multiple factors could influence the supplier decision, a key factor that might be considered is the profitability or the return on investment. Accordingly, the agent could autonomously make decision on whether to expand the production capacity and if so by how much, which will impact other modules and other agent decisions. A pseudocode is provided below in to show how this was implemented in the model. It shows the implementation of autonomous decision-making regarding capacity expansion decision by the *Fuel Supplier* agent for a given target profit margin and growth rate factor. In a similar way, autonomous decision making can be incorporated within other agents such as the *Airlines* and *Aircraft Manufacturer* agents. Potential avenues to consider include decisions regarding the manufacturing and purchasing of LH2 based aircraft, capacity of the fleet, level of investment in technology development, and so forth.

VI. CONCLUSION AND DISCUSSION

A hybrid modular SD and ABM model is presented for the analysis of the adoption of sustainable fuels, and supply and demand tension, considering perspectives of different stakeholders such as airlines, airframe integrators, feedstock suppliers, processing chains, production and logistics infrastructure developers, policymakers, and regulatory authorities. The complex dynamics arising from the interaction of these diverse actors require a sociotechnical system model at scalable abstraction to capture strategic decisions at high simulation speed using the SD approach. The modular SD approach enables integration while also allows zooms in on the low-level details for parametric determinations of exact system operationalization in terms of costs, delays, and sizing. The mid-abstraction method of ABM enables SD modules to be represented as interacting agents with their unique local behaviors and autonomous decision making. These modeling features are advantageous in calibrating and validating the model to a particular stakeholder's needs. The practical relevance of such frameworks is significant. The study intends to provide industry stakeholders and policymakers with a tool to understand the complex interactions and feedback loops that drive the development and subsequent market adoption of a new fuel technologies. Furthermore, by simulating various scenarios, including potential disruptions, this model will help to visualize the dynamic relationships between inputs and outcomes thereby enabling strategic planning and helps de-risk the substantial investments required in technology transitions. These modeling and simulation developments will therefore provide quantitative insights into the challenges and enablers of sustainable fuel adoption, helping to guide aircraft manufacturers, airlines, airports and policy makers.

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