Airline Decision-Making in Sustainable Aviation Fuel Transition: A Hybrid Simulation Modeling Approach

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***Abstract*—This study presents a hybrid simulation approach combining Agent-Based Modeling (ABM) and System Dynamics (SD) to capture the evolving system behavior through interacting stakeholders, including airlines, manufacturers, airports, and fuel suppliers, and to analyze how airlines adopt sustainable aviation fuels within the broader transition of the Air Transportation System (ATS). Because the existing models often overlook the interplay between micro- and macro-level dynamics, this study addresses that limitation by integrating both agent-level behaviors and broader systemic trends, such as passenger demand, Gross Domestic Product growth, and infrastructure constraints. SD captures the internal agent dynamics using stocks and flows, for example, passenger demand shaped by societal and economic trends. The ABM architecture represents each airline as an agent, modeled as a key decision-maker that monitors demand and capacity dynamics and makes strategic investment decisions in aircraft and fuel technologies. It is designed to represent how airlines implement and adjust their strategies in response to internal factors including various operational aspects and external factors including infrastructure support and sustainable fuel availability. Integrating ABM and SD enables concurrent simulation of agent-level behaviors and system-level feedback, providing a comprehensive view of the sociotechnical components in the ATS and their decision-making.**

Keywords-Air Transportation System; Hybrid Simulation; Sustainability; Agent-Based Modeling; System Dynamics.

I. INTRODUCTION

As climate change is becoming an emerging critical global challenge, the aviation industry has committed to achieving net zero CO_2 emissions by 2050 [1]. Achieving this goal requires various technical and operational measures within Air Transport Systems (ATS) [2], including the adoption of more sustainable fuels and advanced aircraft technologies compatible with these fuels with improved energy efficiency. Furthermore, enabling the transition from kerosene-based fuels to sustainable fuels involves the establishment of supporting energy infrastructure, including both the fuel technologies and the systems required for their deployment, production, storage, and distribution. To date, Sustainable Aviation Fuel (SAF), liquid hydrogen (LH_2), ammonia (NH_3), and methanol (CH_3OH) are considered as the potential sustainable fuel options for increased sustainability, each with its own characteristics in terms of technological maturity, scalability, environmental benefits, and transition challenges.

To understand the gradual transition of the ATS from keronese-based fuels to sustainability comprehensively, as characterized by the complex sociotechnical interactions and dynamic behaviors, it is important to adopt methodologies that can effectively capture inter-dependencies of different components within the system and their impacts on the overall system. Simulation-based methods, including Agent-Based Modeling (ABM) and System Dynamics (SD), are considered powerful tools for examining and explaining the key mechanisms and interactions within complex sociotechnical systems, to support the design and analysis of such systems [3]. ABM is used to simulate the behavior of the emerging system from the interactions of autonomous agents [4], while SD models the evolution of the system driven by feedback using causal loop diagrams and stock flow simulations [5]. Both are widely used for modeling complex, dynamic systems and support "what-if" analysis without real-world intervention [6].

The central objective of the present work is to study how airlines make strategic decisions about adopting more sustainable aviation fuels. Despite rising interest in sustainable transitions, hybrid simulations combining ABM and SD remain underexplored. Most existing studies either employ ABM or SD in isolation, and therefore miss the micromacro interplay which is important for fleet-transition planning that involves complex interactions among industry stakeholders, market forces, and policy measures [6][7]. To address this gap, this paper proposes a novel hybrid simulation approach that combines ABM and SD to model airline decision-making processes in sustainable aviation transitions.

The study aims to capture the complex interactions among technology, industry, markets, and society, and to simulate airline decision-making processes related to the acquisition of new sustainable aircraft. ABM and SD methods are complementary and can be integrated effectively; however, despite the feasibility, such integration remains rare and has limited application [7]. ABM uses a micro-modelling approach, focusing on the behavior of individual agents, while SD uses a macro-modeling approach, focusing on the aggregated stocks and flows that represent higher-level or broader population-level dynamics [7]. Both are relevant and valuable for analyzing the aviation transition to more sustainable fuels. The hybrid ABM and SD approach allows for a more comprehensive and realistic representation of the sociotechnical elements within the ATS, their interactions, and decision-making processes. It enables capturing relevant elements of individual heterogeneity and stochasticity of entities and processes [6], such as micro-level decision behaviors (e.g., individual airline strategies), while also providing a strategic overview [6] of macro-level system impacts (e.g., population and GDP trends) for estimating passenger demand, manufacturer capacity, government support, and infrastructure constraints. This study makes four key contributions. First, it introduces a conceptual architecture for a hybrid simulation of the ATS that unifies SD and ABM principles, providing a clear, holistic picture of how macro-level stocks-and-flows and micro-level agents interact in a single framework. Second, the paper specifies the SD side in-depth, elaborating the governing equations and feedback loops for core modules, such as fleet capacity, passenger demand, and environmental constraints, and showing how these modules shape aggregate system behavior over time. Third, it sets out a rigorous ABM methodology that captures the behavior of airlines, airports, regulators, and passengers. Special emphasis is placed on the airline decision logic for scheduling, pricing, and fleet deployment, thereby grounding the model in realistic operational choices. The work describes an explicit macro-to-micro coupling strategy that synchronizes SD state variables with ABM agent states, ensuring internal consistency and enabling the exploration of emergent phenomena across multiple temporal and organizational scales. Collectively, these advances deliver a reproducible blueprint for researchers who wish to combine SD and ABM when analyzing complex socio-technical systems, such as the ATS.

The paper is organized as follows. The overall framework is presented in Section II. Within this, the high-level SD modeling for *Society* and *Airlines* agents are outlined in Section II-A. The focus then shifts in Section II-B to the Agent-Based Modeling that governs airline decision-making. The paper concludes in Section III with a discussion of applications and future work.

II. Hybrid ABM-SD Conceptual Framework

The conceptual framework illustrating different sociotechnical elements considered in this study is shown via Figure 1. The figure provides a high-level view of interacting agent components of the ATS, including *Society, Airlines, Aircraft Manufacturer, Airport* and *Fuel Supplier*, and their underlying SD modules, forming the conceptual structure of the simulation model.

Within each agent's block are the names of the specific SD modules that represent that agent's internal dynamics. The agents are connected by arrows illustrating the key flows and dependencies and indicating how agents interact and influence each other. The framework highlights the holistic view of the system and shows how the interactions between various sociotechnical elements within the ATS together shape and drive the overall dynamics and evolution of the sustainable fuel transition. By modeling these key actors as interacting agents, the framework allows for capturing emergent system behaviors that arise from the bottom-up interactions of individual components, providing a powerful mechanism to analyze the complex pathways and challenges of aviation transition.

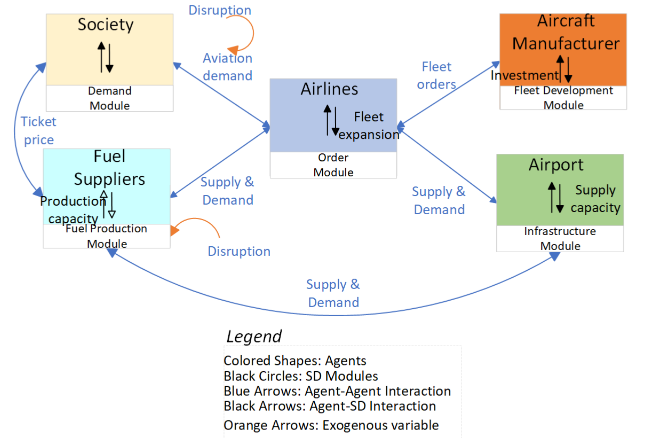

Figure 1. Hybrid ABM-SD conceptual framework of the ATS.

A. System Dynamics Modeling: Stock and Flow Diagrams for Society, Airlines, and Aircraft Manufacturers

The stock and flow diagrams were created to capture the feedback structure within the *Society, Airlines*, and *Aircraft Manufacturer* agents.

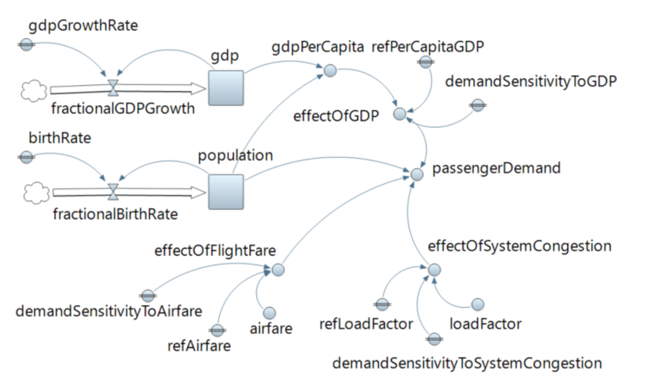

Figure 2. Stock and flow diagram of the *Society* agent

The stock and flow diagram shown in Figure 2 illustrates the core dynamics of the passenger demand module within the *Society* agent, which aims to simulate passenger demand and takes into account several key determinants of demand as contributing factors. Multiple factors have been identified in the literature that directly or indirectly influence aviation passenger demand; however, at a broad level, they can be differentiated into two categories: internal determinants and external determinants. The internal determinants of demand mostly cover the service level aspects of the service providers, including airlines and airports, and thus are related to passenger perception; whereas, the external determinants comprise demographic and geo-economic factors of a region [8][9]. Amongst all these, ticket prices, system congestion, population, and income of the population are selected as these have been considered important and utilized to estimate aviation demand in the literature [10]–[13]. To represent the effect of population income on demand, gross domestic product (GDP) per capita is employed as a common indicator of average income level within a population [14]. These dynamics are captured in the stock-and-flow structure, which includes two key stocks: the GDP stock representing GDP and influenced by the GDP growth rate; and the population stock, representing the total population of a region, which increases through the birth flow determined by the birth rate. The relationship is as follows:

$$p = K \times \gamma_{\text{gdp}} \times \gamma_{\text{sc}} \times \gamma_{\text{fare}} \tag{1}$$

where p denotes total aviation demand, K represents population size, and γ denotes effect of different factors. The relation used to estimate factors, such as the effect of GDP, system congestion, etc., is as follows:

$$\gamma_{\text{gdp}} = \left(\frac{A(t)}{A}\right)^{\alpha} \tag{2}$$

where the fraction represents the ratio of the current value (at time t) of the variable with respect to the reference value, and α denotes the sensitivity factor of the quantity at hand.

Figure 3 depicts the internal dynamic processes within the *Airlines* agent. The stock, represented by the 'operationalFleet' variable, represents the number of aircraft currently in service. Within this model, the overall fleet is divided into two subcategories based on the fuel type they may be able to utilize, *i.e.* the kerosene-based aircraft and the more sustainable fleet or non-kerosene-based aircraft. Moreover, within each category, the aircraft are further classified into the following types: 1) short distance, 2) medium distance, and 3) long distance, based on the flight haulage. The categorization is crucial as the seating capacity is different for each of these aircraft types. These distinctions are hereafter referred to as fuel-based and distance-based classifications.

The fleet of the airlines is increased by the addition of newer aircraft procured from the manufacturer, and the rate of increase is determined by the 'orderFulfillmentRate' variable. On the other hand, the 'operationalFleet' decreases due to aircraft 'retirement' flow, governed by the retirement rate (indicated by 'retirementRate' variable in Figure 3). Furthermore, as seen in the figure, Available Seat Kilometers (ASKs) and Revenue Passenger Kilometers (RPKs) are computed. Both these quantities are important metrics utilized by airlines to track their operational performance. ASKs are tracked by airlines to measure their total passenger carrying capacity, and RPKs are utilized to assess the volume of passengers carried by them [15]. These metrics are obtained by using the following relations:

$$\text{ASK}_d = n_d \times c_d \times s_d \tag{3}$$

$$\text{RPK}_d = p_d \times s_d \tag{4}$$

where d = {short, medium, long} and corresponds to different flight distance categories; n is the number of operational aircraft; c represents the capacity or the number of seats; s is the average flight distance; and p corresponds to the demand for the d type of aircraft, obtained by multiplying the proportion of demand for each flight category with the total demand.

Subsequently, ASKs and RPKs are used to generate the passenger load factor (PLF) which is defined as the proportion of available seats filled with passengers [15] and computed using the following relation:

$$\text{PLF}_d = \frac{\text{RPK}_d}{\text{ASK}_d} \tag{5}$$

This metric is subsequently utilized for the estimation of the total traffic intensity factor. Revenue is estimated as a function of traffic intensity, RPKs, and the average passenger yield is categorized according to flight distance. Profit is computed with revenue and costs as the contributing factors. The overall airline's costs are determined by the aggregation of various cost components, specifically fuel costs, operating costs, and penalty costs. Furthermore, a penalty is imposed as an external cost due to deviation from the sustainability target. In other words, airlines need to maintain a specific proportion of a more sustainable fleet, and when there is a shortfall in the target, a penalty is charged. Airline decision on new aircraft orders is governed by the interaction of variables representing fleet capacity and the target capacity. When the existing capacity falls below a pre-specified threshold level, orders are placed to the *Manufacturer* agent. This order management is handled by the agent architecture and is discussed in the next section.

The primary function of the SD module within the *Manufacturer* agent is to process orders and deliver fleet to the *Airlines* agent. As observed from Figure 4, there are two stocks in the figure: 'orderStock', which represents the backlog of aircraft orders received from the airlines and waiting to be manufactured. The production rate is controlled by the capacity variable. 'finishedOrders' stock variable accumulates the aircraft that have been manufactured and are ready for delivery. This information is then utilized to apprise the manufacturer about the delivery of aircraft. Conceptually, the figure outlines orders entering a backlog (orderStock), being processed through production (reducing order stock and increasing finished orders stock), and finally being delivered. The rates of production and delivery are constrained or influenced by the manufacturer's capacity.

B. *Agent Based Modeling: Airlines Decision Making*

Agent-based models are composed of individual agents, each with its own behavior, states, interaction protocols, and decision-making rules. Elements or components of the ATS are classified as passive agents and active agents. Both of these agent types share common features: they are autonomous, self-directed, interactive, and have explicit goals. Their key distinction lies in their decision-making ability; an active agent can learn and adapt its behavior in response to a change in the environment. Therefore, the *Society* agent can be categorized as a passive agent while the *Airlines* and *Manufacturer* agents are modeled as active agents.

As a passive agent, the primary purpose of the *Society* agent is to simulate the passenger demand which has been described in Section II-A; the generated demand is then communicated to the *Airlines* agent. Meanwhile, as an active agent, the *Airlines*

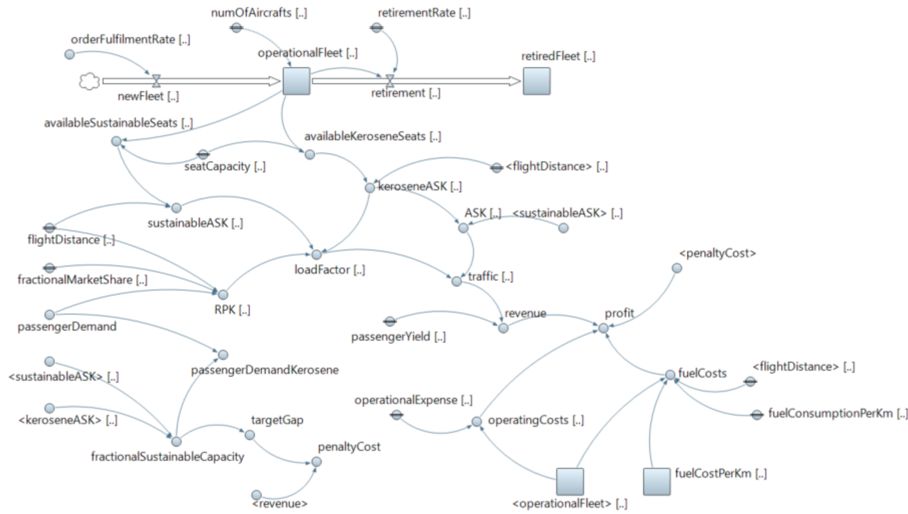

Figure 3. Stock and flow diagram of the *Airlines* agent.

agent compares the demand against the capacity. When the capacity-to-demand ratio reaches a specific threshold, a new order is placed.

The order-making process for selecting appropriate aircraft and fuel technology is grounded and structured on two key factors, including internal and external factors. The internal factors are those that pertain directly to the airlines' own operational context and priorities and reflect internal considerations. J is a set of different fuel technologies modeled in the paper, and J= {Kerosene, SAF, NH_3, CH_3OH, H_2}, indicating different fuel technologies. Furthermore, internal factors are denoted using θ and external factors using ϕ notations, respectively. Also note that both, θ & $\phi \in [0, 1]$. The internal factors, described in detail below, relate to variables intrinsic to the *Airlines* agent, reflecting operational or strategic considerations that influence decision-making.

1) Operational cost factor (θ^{oc}): This factor focuses on "per flight cost", encompassing both variable and fixed cost components of different aircraft types. The operational costs are represented with $C = \{c_j | j \in J\}$, and the operational cost factor for a flight of type j is computed using the relation:

$$\theta_j^{oc} = \frac{\min\{C\}}{c_j} \tag{6}$$

The aim is to select the aircraft with lower operational expenditures, therefore, the operational cost score is calculated to reflect this, where a higher score would typically be assigned to options with lower costs. The expression is used as it

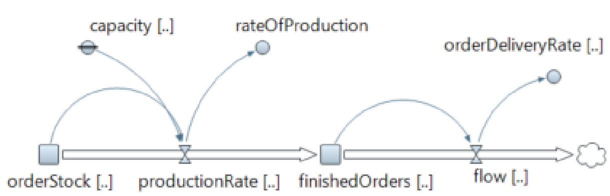

Figure 4. Stock and flow diagram of the *Manufacturer* agent

normalizes the cost of an option j against the minimum achievable cost, rewarding lower-cost options.

2) Operational life factor (θ^{ol}): Similar to the previous metric (discussed in section II-B1), this factor is used to capture the impact of the operational life of the aircraft. It is a relative score that is designed to assign a lower value to aircraft with shorter operational life and vice versa, as expressed below:

$$\theta_j^{ol} = \frac{\min\{L\}}{l_j} \tag{7}$$

where $L = \{l_j | j \in J\}$ representing life in years.

3) Sustainability gap factor (θ^s): A key consideration included in the decision-making process accounts for the airlines' performance against sustainable fleet targets. It specifically measures the gap between the actual proportion of sustainable fleet ASKs and the targeted proportion for a given period. It is to be noted that this factor adds extra weight to the score of non-kerosene-based aircraft. Thus, it is estimated using the relation:

$$\theta_j^s = \begin{cases} 0, & \text{if } j = \text{kerosene} \\ 1 - \min\left(\frac{f(t)}{f}, 1\right), & \text{otherwise} \end{cases} \tag{8}$$

where f stands for the sustainability target and $f(t)$ is a function of time and indicates the current proportion of non-kerosene-based aircraft.

These internal factors are then combined to calculate the total internal score for all the available aircraft options.

$$\theta_j = \theta_j^s + \theta_j^{ol} + \theta_j^{oc} \qquad \forall j \in J \tag{9}$$

The external factors are those which are external to the *Airlines* agent and concern the wider air transportation ecosystem. These factors, specifically, originate and depend on *Manufacturer*, *Airport*, and *Fuel Supplier* agents.

4) Order delivery factor (ϕ^M): This factor is specific to the *Manufacturer* agent. It assesses the manufacturing landscape by weighing in the expected delivery time of the aircraft order. The *Airlines* agent interacts with the *Manufacturer* agent to retrieve the order delivery time frame. A long order delivery time will translate to a lower value of the order delivery factor for that particular aircraft type. This factor is derived using the formula:

$$\phi_j^M = \frac{\min(T)}{t_j} \tag{10}$$

where $T = \{t_j | j \in J\}$ denotes time.

5) Infrastructure support factor (ϕ^{Infra}): The support infrastructure factor is available for a given fuel technology, in terms of fuel delivery and storage, both currently and in the future. The idea is to give more weight to technologies with better infrastructure with potential for future development. Consequently, this factor has two distinct components: 1) present (ϕ_p) and 2) future (ϕ_z), and is obtained using the relation:

$$\phi_j^{\text{Infra}} = w_1\phi_j^p + w_2\phi_j^z \tag{11}$$

where p and z denote present and future, respectively; and w_1 and w_2 are the weights that sum to 1 and denote the relative importance of these components. The score for the present state of the infrastructure support is calculated by considering the capacity utilization level, with a higher score assigned to lower capacity utilization values because of its capacity to accommodate more demand.

$$\phi_j^p = 1 - \rho_j \tag{12}$$

Where ρ_j indicates the utilization level of technology j. The future aspect is included to factor in the prospects of growth in a specific technology. For example, a higher relative investment in hydrogen technology signifies stronger future support and development, leading to a higher score.

$$\phi_j^z = \frac{Q_j}{\sum_j Q_j} \tag{13}$$

In this case, Q is the notation to indicate investment.

6) Fuel Supply Factor (ϕ^{FS}): This factor covers the supply side for different fuel types, considering the current availability and, the future growth prospects. This encompasses the assessment of how readily the fuel can be sourced now and the long-term outlook and the development of the fuel technology. Technologies that are relatively secure and scalable would be rated relatively favorably. Similar to the previous case, the fuel supply factor can be expressed as the weighted sum of the present availability (denoted as ϕ^{av}) and future growth potential (denoted as ϕ^{fp}), as presented:

$$\phi^{FS} = w_1\phi_j^{av} + w_2\phi_j^{fp} \qquad \forall j \tag{14}$$

where w_1 and w_2 are weights and sum to 1.

The current fuel availability is obtained by taking into account the fuel production capacities of all the different types of fuel. The following expression is used to obtain its value:

$$\phi_j^{av} = \frac{\kappa_j}{\max(\kappa)} \tag{15}$$

where κ indicates the current fuel production capacity.

Next, the prospect corresponds to the capital invested or the planned capital investment in the development of a technology. This factor is calculated by taking a ratio of capital invested in a specific technology and the total capital invested across all the technologies.

$$\phi_j^{fp} = \frac{I_j}{\sum_j I_j} \tag{16}$$

Here, the notation I is employed to refer to investment in fuel technologies. The external factors are then summed up to calculate the total external score for all the available aircraft options using the relation:

$$\phi_j = \phi_j^M + \phi_j^{\text{Infra}} + \phi_j^{FS} \qquad \forall j \tag{17}$$

After which, the internal and external factor scores are combined for different aircraft alternatives to estimate the aggregated score, and the option with the maximum score is selected. The entire decision-making procedure is explained using a pseudocode shown in Algorithm 1 via Figure 5. Furthermore, individual calculations of internal and external factor scores are implemented via functions which are presented using Algorithm 2 in Figure 6.

```
procedure AIRLINES AGENT AIRCRAFT TECHNOLOGY SELECTION PROCEDURE
    Determine the required aircraft category‘ (e.g., short, medium, long haul)
    Identify the set of fuel technologies (J) available for the required aircraft category
    Set ‘bestSelectedTechnology‘ ← NULL
    Iterate and Evaluate Technologies:
    for j ∈ J do
        internalScore ← CALCULATEINTERNALSCORE(j)
        externalScore ← CALCULATEEXTERNALSCORE(j)
        aggregatedScore ← internalScore + externalScore
        ’bestSelectedTechnology‘ ← max{internalScore + externalScore}    ▷ Identify the technology with the highest score and update.
    end for
    Decision and Action: Place an order for an aircraft of required aircraft category of the ’bestSelectedTechnology’type
end procedure
```

Figure 5. Algorithm 1: *Airlines* agent decision making procedure.

III. CONCLUSION AND FUTURE WORK

The hybrid ABM-SD frame provides a means to analyze how policy instruments or market shocks propagation through tightly coupled technical and behavioral system elements that ABM or SD alone can capture. The framework lays the analytical groundwork for rigorous, whole-system assessments of sustainable aviation strategies. It offers researchers, industry stakeholders, and policymakers an extensible tool to explore how heterogeneous decision-makers, emerging aircraft technologies, and evolving fuel infrastructures interact over the multi-decade horizon that separates todays fleet from a genuinely low-carbon future. By embedding explicit sustainability gap and penalty mechanisms, the framework offers a transparent way to test how airlines might schedule fleet

Input: $C \in$ {Cost}, $L \in$ {Operational Life}, $T \in$ {Order delivery time}, $\rho \in$ {Infrastructure capacity utilization}, $Q \in$ {Investment in infrastructure development}, $K \in$ {Fuel production capacity}, and $I \in$ {Investment in fuel technology development}, $f \in$ {Sustainability gap}, $w = \{w1, w2\}$, $w' = \{w'_1, w'_2\}$, and t represents simulation time.

function CALCULATEINTERNALSCORE(j)
 $\theta_j^{oc} \leftarrow \frac{\min\{C\}}{C[j]}$ ▷ Operational cost factor
 $\theta_j^{ol} \leftarrow \frac{\min\{L\}}{L[j]}$ ▷ Operational life factor
 θ_j^{s}
 if $j \equiv kerosene$ **then**
  $\theta_j^{s} \leftarrow 0$ ▷ Sustainability gap factor
 else
  $\theta_j^{s} \leftarrow 1 - min\left(\frac{f(t)}{f}, 1\right)$
 end if
return $\theta_j^{oc} + \theta_j^{ol} + \theta_j^{s}$ ▷ Return internal factor score
end function

function CALCULATEEXTERNALSCORE(j)
 Order delivery factor, $\phi_j^{M} \leftarrow \frac{min\{T\}}{T[j]}$
 $\phi_j^{p} \leftarrow 1 - \rho[j]$ ▷ Infrastructure level factor
 $\phi_j^{z} \leftarrow \frac{Q_j}{\sum Q}$ ▷ Infrastructure investment level factor
 $\phi_j^{\text{Infra}} \leftarrow w_1 \times \phi_j^{p} + w_2 \times \phi_j^{z}$ ▷ Infrastructure support factor
 $\phi_j^{av} \leftarrow \frac{\kappa}{\max(\kappa)}$ ▷ Fuel supply availability factor
 $\phi_j^{fp} \leftarrow \frac{I_j}{\sum_j I_j}$ ▷ Fuel supply investment factor
 $\phi_j^{FS} \leftarrow w'_1 \times \phi_j^{av} + w'_2 \times \phi_j^{fp}$ ▷ Fuel supply factor
return $\phi_j^{M} + \phi_j^{Infra} + \phi_j^{\text{FS}}$ ▷ Return the external factor score
end function

Figure 6. Algorithm 2: Functions for calculating *Airlines* agent internal and external factor scores for decision making.

renewal in response to decarbonization targets. The modular structure facilitates scenario experimentation, allowing researchers and practitioners to interchange empirically calibrated sub-models (e.g., refined fuel-supply curves or airport capacity modules) without re-engineering the whole system. The current implementation employs stylized parameters for infrastructure utilization, investment, and fuel production, and systematic calibration with historical airline, manufacturer, and energy-market data would strengthen predictive validity. The future work would aim to expand the models analytical boundaries by implementing active-agent logic for airports and fuel suppliers to enable the simulation of richer, co-dependent strategies, including the effects of slot constraints and supplier learning curves. Next, the model would be integrated with the wider energy infrastructure to simulate the cross-sectoral competition for key inputs, such as electricity and hydrogen, to identify potential risks and macroeconomic bottlenecks. Finally, coupling the model with optimization or reinforcement-learning techniques could support the design of adaptive policy portfolios that steer the ATS toward net-zero trajectories.

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