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Agent-Based Simulation of Integrated Process and Energy Supply Chains: A Case Study on Biofuel Production

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ABSTRACT

Despite the potential benefits of decision-level integration for process and energy supply chains (SCs), these systems are traditionally assessed and optimised by incorporating simplified unit operation models within a spatially distributed network. The desired organisational-level integration cannot be achieved without leveraging complex computational tools and concepts. This work proposes a multi-scale agent-based model to facilitate the transition from traditional practices to coordinated SCs. The proposed multi-agent system framework incorporates different enterprise dimensions of the process and energy SCs, including raw material suppliers, rigorous processing plants, and consumers. The behaviour of each agent type and its interactions are implemented, and their impact on the overall system is investigated. This approach allows for the simultaneous assessment and optimisation of process and SC decisions. By integrating each decision level into the operation, the devised framework goes beyond existing studies in which the impacts of lower decision levels are neglected. A biofuel SC example comprising farmers, biorefineries, and end-users is presented to demonstrate the application of the proposed multi-agent system. The involved actors seek to increase their payoffs given their interdependencies, intra-organisational variables, and the underlying dynamics of the network. The aggregated payoff of the supply network is optimised under different scenarios, and fractions of capacity allocated to biofuel production and consumption are obtained. The results indicate that integrated decision-making significantly influences SC performance. The proposed research expounds a more realistic view of multi-scale coordination schemes in process and energy SCs.

Keywords: Process and energy systems, Decision level integration, Agent-based models, Biofuel supply chains, Payoff optimisation

INTRODUCTION

Effective coordination between supply chain (SC) levels from operational to strategic areas is an essential tool for improving the comprehensiveness of process and energy system models [1]. Such a decision-level integration notion is true for models encompassing changing policy decisions and technological innovations, such as those in biofuel SCs [1]. Biofuels can provide an essential alternative to fossil fuels as they utilise renewable feedstocks whilst allowing for lower net carbon dioxide emissions [2]. Although the further adoption of biofuels has been touted as a possible key contributor to meeting the climate objectives, the complex interactions between stakeholders, such as raw material suppliers, processing plants, and consumers, and the impact of government policies, such as subsidies, result in unclear or oversimplified outcomes from conventional biofuel SC models.

Several studies have explored the optimisation of biofuel SCs to meet sustainability objectives [3-5]. Whilst some explore the impact of technology options on SCs, none were found to investigate the effects of biorefinery process details on biofuel adoption. In this context, computational approaches such as agent-based modelling have been used to handle the complexities and uncertainties associated with biofuel SCs, specifically the feedback relationships between agents [1]. The most rigorous studies [1, 6], proposed agent-based models to simulate the adoption of biofuels by stakeholders in response to government policies such as differing subsidy

levels and products' social and environmental impacts. The current investigation utilises a multi-scale agent-based model to capture the organisational structure of integrated SCs. Such multi-faceted features allow for simultaneous assessment and optimisation problems, particularly exploring the optimal adoption in biofuel-driven processes and energy systems. The framework extends decision-making beyond that from prior studies by including decisions at the firm level, through adjustments to intra-organisational planning options, as well as at lower levels, through the incorporation of biorefinery process variables.

METHODOLOGY

Biofuel Adoption Problem Formulation

In this work, a biofuel SC is modelled as an interrelated system of computational ecosystems featuring distributed and asynchronous decision-making, and incomplete information. The conceptual structure of the system is shown in Figure 1.
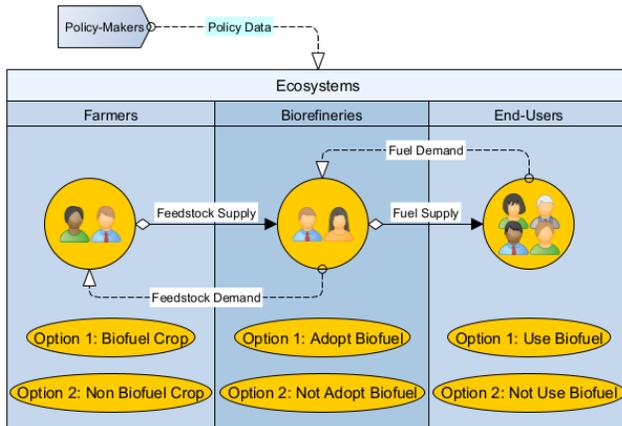
Figure 1. Conceptual model of the biofuel SC [1].

The system comprises multiple actors, including farmers, biorefinery facilities, and end-users, each with binary options regarding biofuel adoption. The biofuel adoption problem is formulated as follows.

$$max_{P,O} \; \mathcal{U}_T = \sum_{e \in SCE} \sum_{t_m \in T_m} \mathcal{U}_t(P, O) \qquad (1a)$$

$$s.t. \; P \in \Theta_P, O \in \Theta_O \qquad (1b)$$

Where $\mathcal{U}_T$ is the total utility of all involved ecosystems (SCE) in all sample periods (T_m), which is calculated by the individual payoff functions ($\mathcal{U}_t(P, O)$). The planning decision variables (P) include re-evaluation frequencies, while the operational-level decisions (O) entail adjusting biorefining facility process parameters. Additionally, the feasible regions of both levels confined by equality, inequality, and implicit constraints are denoted by sets Θ_P and Θ_O.

Supply Chain Dynamic Behaviour

The SC behaviour at the aggregate level is driven by actors alternating between adopting or not adopting biofuels and changing the ecosystem's payoff. The following constraints determine the rate at which actors choose the former at the ecosystem level [1].

$$\frac{df_e}{dt} = \alpha_e \left(\rho_e \big(f_i(t - \tau_e) \big) - f_e(t) \right), \forall e, i \in SCE \qquad (2)$$

$$\rho_e = \frac{1}{2} \left(1 + \text{erf} \left(\frac{G_{e1}(f_i) - G_{e2}(f_i)}{2\sigma_e} \right) \right), \forall e, i \in SCE \qquad (3)$$

$$\alpha_e \in (\alpha_{e,min}, \alpha_{e,max}) \qquad (4)$$

Where f_e is the fraction of actors in an ecosystem adopting biofuels and α_e [$\frac{1}{month}$] is the re-evaluation frequency for each ecosystem, bounded by minimum and maximum values ($\alpha_{e,min}, \alpha_{e,max}$). The preference probability of biofuel adoption (ρ_e) depends on the payoff of selecting said option. As a result, two utility functions, represented as G_{e1} and G_{e2} are defined for adopting or not adopting biofuels, respectively, influenced by same-tier and neighbouring ecosystem adoption fractions. τ_e denotes the delay parameter and accounts for the asynchronous information flows between ecosystems and the inherent inertia to respond to external changes. Finally, the uncertainties are introduced through measurement errors of utility functions, characterised by σ_e [1].

Biorefinery Model

The production process behaviour is reflected via a nonlinear model of a biodiesel plant described elsewhere [7]. The closed form of the process model is described below.

$$\mathcal{F}(\mathcal{X}) = 0 \qquad (5)$$

$$x \in (x_{min}, x_{max}), \forall x \in \mathcal{X} \qquad (6)$$

Where $\mathcal{X}$ refers to the process variables and parameters, including feed and solvent flow rates and temperatures along with water mass flow and the boiler pressure. The set $\mathcal{F}$ relates the final product flow rate, purity, temperature, and heat duty requirement to the input parameters [7].
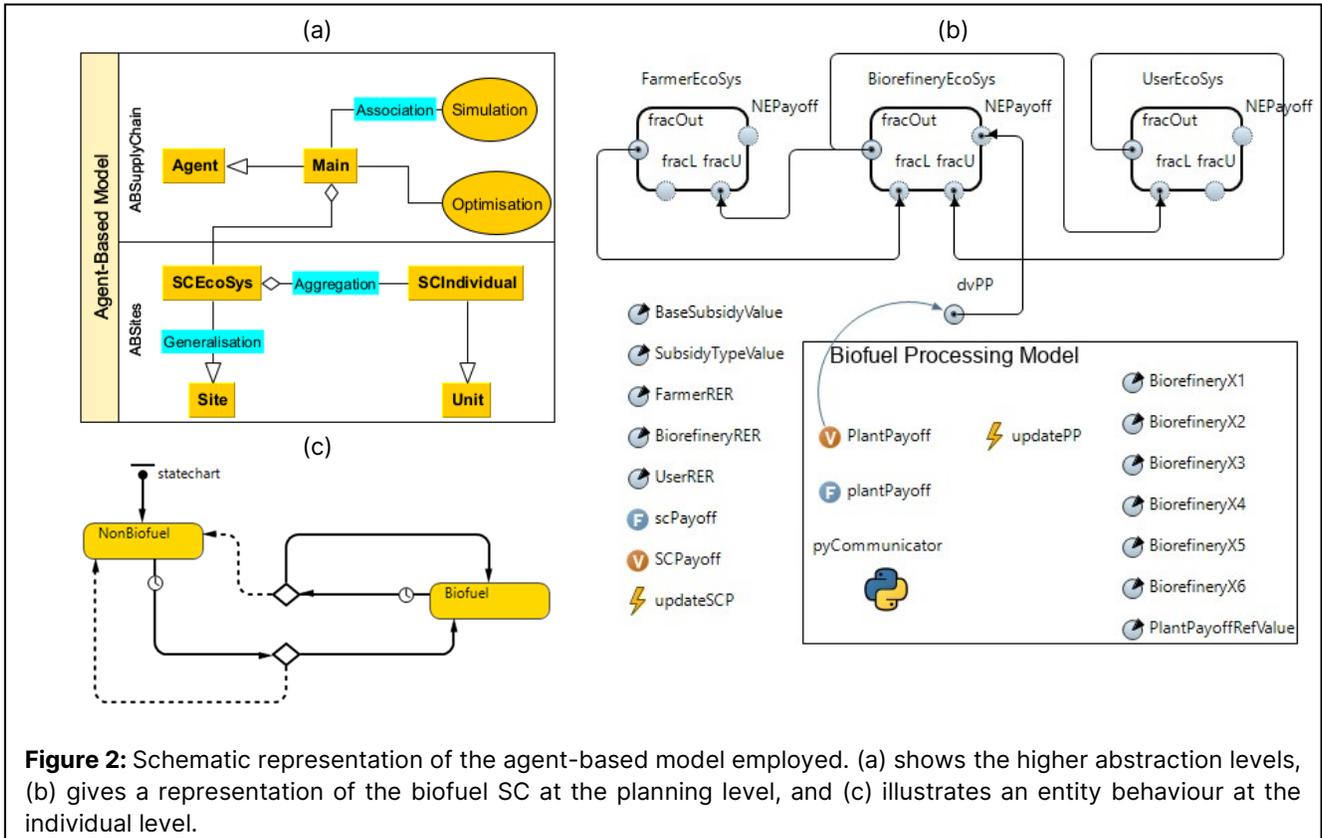
The plant's overall profit is calculated based on the following equation.

$$Profit = Sale_{Biodiesel} - TAC \qquad (7)$$

Where $Sale_{Biodiesel}$ represents the final product sale, and TAC refers to the total annual costs, which include the operational and annualised capital costs discounted by a given factor.

Multi-Scale Agent-Based Model

A multi-agent system encompasses various actors carrying out numerous tasks. These agents can select from multiple resources to complete their assignments.

Figure 2: Schematic representation of the agent-based model employed. (a) shows the higher abstraction levels, (b) gives a representation of the biofuel SC at the planning level, and (c) illustrates an entity behaviour at the individual level.

Their choices are based on the perceived benefits of each resource. While these decisions are rational, they may not always result in the best overall performance for the system. Due to these similarities, the agent-based modelling approach is selected to reflect the complex process and energy systems. The framework materialises a two-level hierarchy by conceptualising and abstracting specific supply networks [1, 8]. For implementation purposes, the AnyLogic software (ver. 8.7.9) [9] is employed due to its ease of use in incorporating different intricacy levels.

Supply Chain Domain Model

Figure 2(a) shows the domain model, in which connections of two broad modules are established. The supply chain module offers the main functionality to represent the overall structure of supply networks. At the same time, the site module involves elements comprising Unit and Site to capture the details of an individual or ecosystem in a network.

Application-Level Model

The specialised model, as illustrated in Figure 2(b), supports the high-abstraction model for the biofuel adoption problem and encompasses three interconnected agents to represent partners of the SC. The framework reflects the two-option behaviour of each component in the system, as demonstrated in Figure 2(c). A linear realisation of coupled payoff functions is used,

similar to the case discussed in the previous investigation [1]. The process model is deployed in Python using Pyomo (ver. 6.8.0) [10] and connected to the main platform via the Pypeline interface.
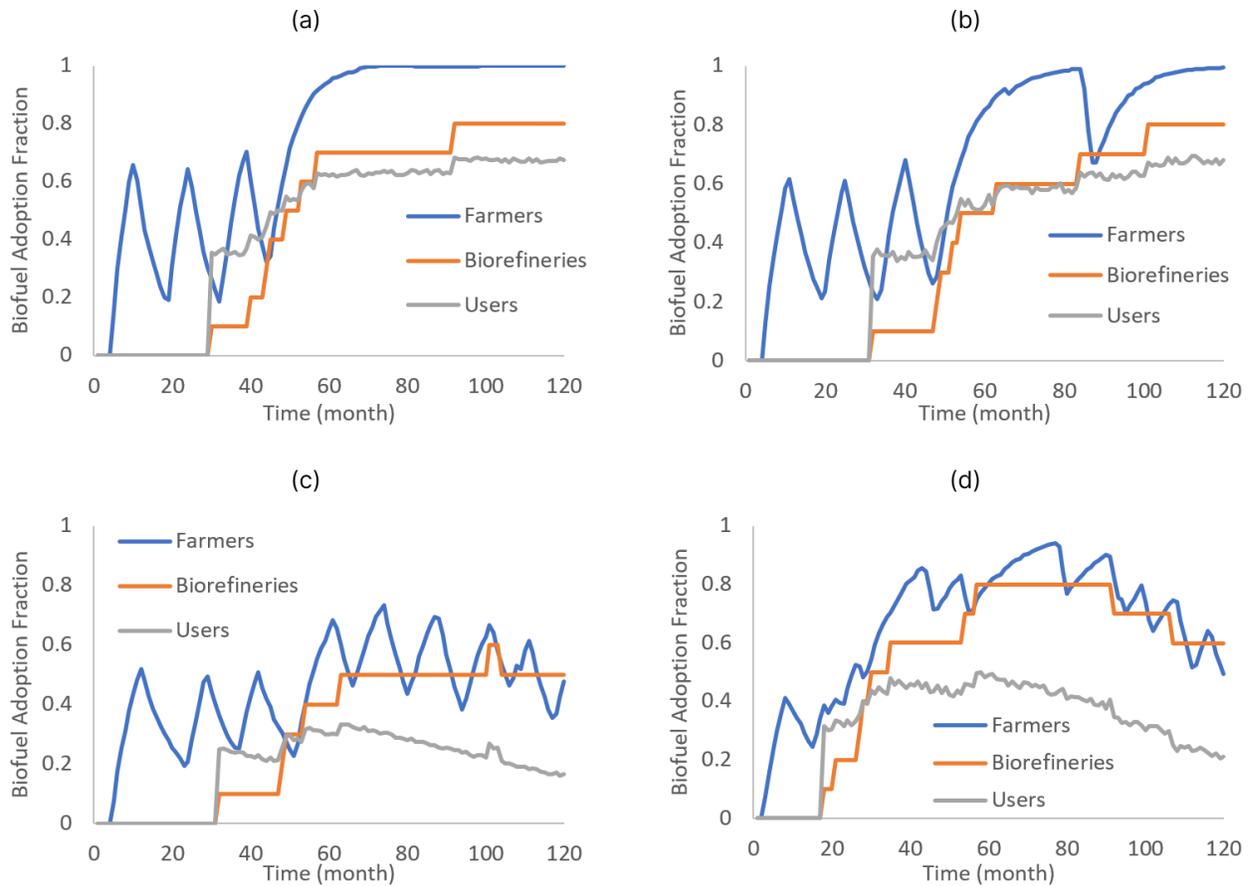
Solution Strategy

The solution strategy is depicted in Figure 3.
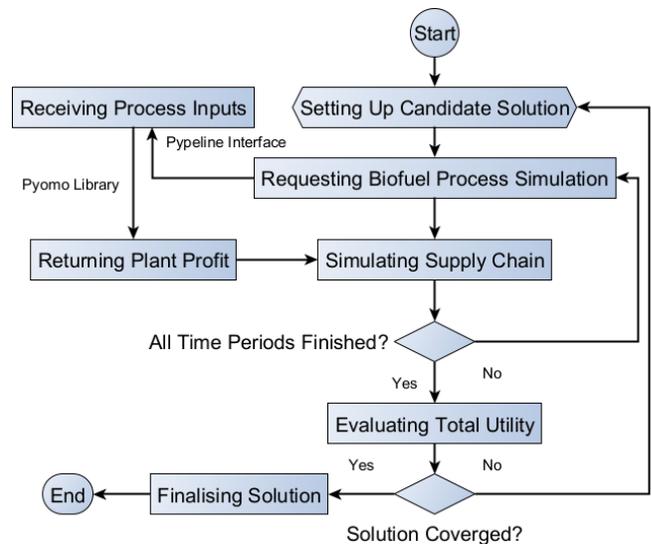
Figure 3. The solution workflow.

As seen in the figure, the optimisation engine creates a candidate solution comprising the re-evaluation

Figure 4: The variation of adoption fraction over time for (a) Scenario 1, (b) Scenario 2, (c) Scenario 3, and (d) Scenario 4.

rates and biofuel process variables and sends it to the corresponding ecosystems. Each ecosystem computes its contribution to the total utility and sends the information to the main agent. For the biorefinery optimisation, process variables are sent to the external Python model, and the obtained profit value is used to scale the respective ecosystem payoff. In this context, the process model is an implicit constraint of the optimal adoption problem. The aggregated utilities are then calculated, and if required, a new candidate solution is generated to be utilised for the next iteration. Notably, without the biorefinery's implicit constraints and under specific conditions with no delays and uncertainties, the optimisation and agent interactions may lead to an equilibrium point (See [1]).

CASE STUDY

A biofuel SC case study is adopted from the prior study [1]. The specific model and parameters for biofuel plants [7] are also incorporated into the optimisation problem. Four scenarios are considered, details of which are summarised in Table 1. As seen in the table, the considered cases are characterised by different subsidy levels or delay parameters (scaled against default values), and the inclusion or absence of the biorefinery considerations (Equations 5-7). Notably, two subsidy types, constant and phased-out policies, are considered. The subsidy values positively affect the payoff of adopting biofuels in each ecosystem. While both types have a similar base value, the latter is in full effect at the start and linearly decreases to zero at the final period [1].

Table 1: Implemented scenarios.

No.	Process Constraints	Subsidy (Base Value)	Delay Scale Factor
1	No	Constant (5)	1
2	Yes	Constant (5)	1
3	Yes	Phased-Out (5)	1
4	Yes	Phased-Out (5)	1/2

The dynamic adoption problem (Equations 1-7), implemented in the AnyLogic environment, is optimised using OptQuest solver across 10 years with monthly sample periods. Ecosystem populations of farmers, biorefineries,

and users are 1000, 10, and 30000, respectively. A maximum of 1000 generations is used as the convergence measure to improve performance, compared to the default criteria. Other considerations, such as raw material and biodiesel prices and bounds for the ecosystem parameters, remain the same as in the prior works [1, 7]. Notably, the existence of delay and uncertain parameters and process constraints pose a serious challenge in reaching and identifying equilibria in discussed scenarios. The implemented scenarios intend to evidence the impacts of decision-level integrations and intricate considerations (delays and uncertainties) on the SC's overall performance. All experiments are performed on an Intel(R) Xeon(R) CPU E5-2620 processor and 128GB RAM.

RESULTS AND DISCUSSION

Figure 4 presents the predicted adoption fraction over time for the different scenarios. In addition, the supply chain decision variables and utility function values are listed in Table 2. In the following sections, the study results are discussed.

Table 2: Scenario results.

No.	$\alpha_{Farmers}$	$\alpha_{Biorefineries}$	α_{Users}	u_T
1	0.165	0.009	12.68	540.31
2	0.13	0.008	26.81	536.15
3	0.089	0.008	7.33	823.24
4	0.083	0.014	18.11	731.63

Influences of The Biofuel Process Model

As seen in Figures 4(a) and 4(b), there is a significant difference in the adoption fraction of actors in the system, particularly in the later time horizons. This comparison indicates the impacts of the biofuel process on SC behaviour. While biorefineries attain similar adoption fractions in both cases, a late accelerated adoption and a subsequent drop (particularly for farmers) can be seen in the second scenario. This observation can be attributed to the fact that processing plant integration enhances the whole environment's visibility, slightly downgrading the actors' participation. In addition, the second scenario features the coupling of raw material supply from farmers and biofuel demand from users. At later planning stages, the increased potential supply of feedstocks creates local competition among farmers, adversely influencing their adoption. The resulting drop has cascading effects on downstream actors, as shown in Figure 4(b).

The same conclusion can be drawn by comparing the objective function values in Table 2, in which incorporating plant constraints leads to a more accurate estimation of the total utility. Here, the changes in SC decision variables are more noticeable, particularly the re-evaluation rates of users. Based on Table 2, due to the introduction of process constraints, users re-evaluate their decisions more frequently. At the same time, other ecosystems assess their decisions less regularly, so emergent and asymmetrical effects on farmers and users can be observed.

Subsidy and Delay Effects

Figures 4(b) and 4(c) show that a constant subsidy leads to higher overall adoption fractions, indicating its effectiveness in promoting consistent adoption. However, the declining subsidy leads to a higher total utility value, owing to the regular changes in the adoption patterns. Therefore, a trade-off between subsidy types and values exists, potentially guaranteeing a less oscillating adoption and higher payoffs.

Scenario 4 has a reduced delay factor compared to Scenario 3. Figures 4(c) and 4(d) reveal that a smaller delay factor results in faster adoption rates, highlighting the importance of information flow and responsiveness in the SC. The reduced information delay also translates to higher adoption fractions across all parties. In contrast, increased information flows lead to a lower utility and a less stable adoption pattern, specifically for biorefineries and end-users.

Overall, Figure 4 and Table 2 provide evidence supporting the argument that biofuel SC models should consider process details, policy types, and information delays to represent system behaviour accurately. These factors directly impact the adoption patterns of different actors, ultimately influencing the success of policy implementation.

CONCLUSION

This work proposes an agent-based framework to explore the multi-scale integration of process plant constraints and the dynamic interactions of multiple actors in the context of process and energy SCs. The developed model implements a bilevel structure to reflect the general and specialised cases such as biofuel SCs. The agent technology effectively captures the interdependencies and feedback relationships among different actors. By accounting for these actors' individual decisions and behaviours, the model provides a more comprehensive representation of the SC dynamics and reveals the potential for emergent system-level behaviours that may not be apparent in simpler models and conventional research works.

The capability of the framework is evidenced via a biofuel SC case study. The SC actors, namely farmers, biorefineries, and end-users, interact in a dynamic network. The case study aims to find an optimal collective adoption pattern based on a two-option strategy at individual levels. Multiple optimisation scenarios featuring

different parameter values and subsidy types are implemented to evaluate the SC aggregated payoff and adoption behaviours. The results show that integrated decision-making leads to a more realistic and insightful biofuel SC model. Integrating process constraints results in a more accurate estimation of the total utility function compared to models that rely on simplified unit operation representations. The findings also underscore the importance of moving beyond the traditional assumption that biorefineries are the sole decision-makers in the SC.

The advantages that arise from this framework extend beyond those mentioned in this study. In this regard, future research should include a better representation of individual payoff functions to capture the intricacies and interactions in biofuel SCs. Furthermore, policy efforts should focus on implementing more complex subsidy types and environmental sustainability measures. By embracing a more holistic and dynamic modelling approach, researchers and decision-makers can better understand the biofuel SC and develop more effective strategies to address the challenges and opportunities associated with this emerging industry.

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