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AI-based Exploration of Socio-technical Safety Barrier Dynamics

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Safety barriers are deployed in a system as a safeguard against undesired events. The prevalent safety barrier concepts focus on component level failures. These concepts may be insufficient for complex systems characterized by limited data & emergent behavior. Recent research developments advocate reframing safety barriers as socio-technical systems, integrating human, organizational, & technical aspects to address emerging risk within the broader context of safety-II & resilience engineering. This study builds on this perspective & investigates the operational safety challenges in a complex hydrogen system. However, quantitative assessment of socio-technical safety barriers is challenging & has not been extensively studied. This study uses synthetic datasets generated from an assumed system dynamics model of a hydrogen refueling station maintenance procedure to demonstrate the feasibility of data-driven identification of socio-technical safety barrier dynamics. These datasets are used for system identification through SINDy algorithm. The two different models are identified with one focusing on interpretability to enable dynamic evaluation of the socio-technical safety barriers & other with focus on predictive performance of the system model. The first model establishes mathematical equations that enable quantitative representation and comparative analysis of socio-technical safety barriers under assumed system dynamics, while second model can be used for predicting & simulating the system dynamics. This approach illustrates the potential to strengthen barrier performance evaluation beyond conventional models. The findings contribute to advancing socio-technical safety barrier analysis methodologies for hydrogen systems, promoting adaptive & resilient strategies.

Keywords: socio-technical safety barriers, emerging risk, hydrogen safety, artificial intelligence, system identification

1. Introduction

Safety barriers were referred to as defenses to serve specific functions in reducing hazards, providing safety guidance, & restoring safety by offering escape & rescue means (Reason, 1997). The literature has presented different definitions of safety barriers (Hollnagel, 2004; ARAMIS, 2004; Sklet, 2006; Subedi et al., 2025). Safety barriers are evaluated based on their functionality, cost, robustness, reliability, response time, & efficiency to prevent, control, or mitigate unintended consequences. The prevalent methods & models to evaluate the safety barriers like safety barrier diagrams, bow-tie diagrams, layer of protection analysis, barrier & operational risk analysis, etc., as summarized by Xie (2022) are limited to data availability & can be insufficient for complex systems (Hollnagel, 2017). Hydrogen systems are complex socio-technical systems (STS) (Pezeshki et al., 2024) & their systemic interactions demonstrate interdependence, complexity, emergence, non-linearity, & adaptability. European Hydrogen Incidents & Accidents database HIAD2.1 (JRC, 2023) indicates 30.3% of recorded hydrogen accidents are caused by human & operational factors. In such a context, traditional assessment methods like human reliability analysis (HRA) would quantify human error probability & try to limit these errors. However, it is essential to understand that decision making ability of an operator could be the very reason for the system to be safe. Furthermore, it is not accurate to evaluate the human factors as independent, rather the assessment of their interaction with the system & the emergence of new behavior can provide better overview of the system dynamics. Recent review study Subedi et al. (2025) has established the need to refine the current understanding of safety barriers with extended definition of safety barriers:

> *Safety barriers are socio-technical systems & can be physical or/and abstract elements that are in place to reduce the potential harm or mitigate the unintended event outcomes; should any component or the system deviate or/and interacts to emerge from its intended function*

The new definition of safety barriers opens possibilities to better understand the dynamicity & complexity of the barriers. It allows to pivot towards reducing risk that may occur from deviations & interactions within the system. This reduces the reliance on past data & predefined understanding. Hence barriers are not static with fixed assessment attributes but rather their role & effectiveness will be defined based on the specific system interaction. This will emphasize system specific assessment & rejection of one-size-fits-all models. Functional resonance analysis method (FRAM) enables the modeling of dynamic & interconnected nature of socio-technical systems to identify emerging risk based on system variability. Subedi et al. (2025) exploited FRAM to introduce socio-technical safety barriers in hydrogen systems. This study deploys the socio-technical safety barriers to reduce the variabilities & hence preventing the deviation of a system from its intended function. Additionally, this study demonstrates the ability of FRAM to determine the performance indicators of socio-technical safety barriers. While the study remained qualitative, the insights from the study established the novel possibility of assessment of socio-technical safety barriers. Nevertheless, the question remains: *Can the dynamic influence of socio-technical safety barriers be quantitatively represented and explored under assumed system dynamics?* In addition to limited data availability, quantification of complex systems is itself challenging as they are characterized as being neither fully knowable nor entirely predictable due to non-linear interactions & emergent behavior (Hollnagel, 2013). This study addresses these challenges by a system dynamics study of hydrogen refueling station. The system dynamics (SD) model is created to produce synthetic datasets for operational procedure involved during maintenance of hydrogen refueling station. The model integrates socio-technical safety barriers & datasets thus produced is assessed to evaluate the barriers quantitatively. The sparse identification of nonlinear dynamical systems (SINDy) algorithm is used to learn a sparse representation of the system's governing equations based on the synthetic data. The results of the SINDy algorithm are then used to evaluate the socio-technical safety barriers & predictive performance of such a data driven approach for SD modeling. In the following section, the contextual background of the study is provided on hydrogen refueling station, socio-technical safety barriers, SD & machine learning (ML) approaches. Then, in methodology, dataset generation & ML model are explained. Finally, the results are presented & critically discussed to make recommendations for further advancement in socio-technical safety barrier assessment.

2. Socio-technical Safety Barriers: Context & Modeling Approach

Hydrogen refueling station comprises several high pressure systems, safety devices, & involves human interaction to maintain its operability & safety. Chauhan et al. (2024) has summarized multiple tasks & sub-tasks involved in maintenance of pressure relief valve within hydrogen fueling station storage unit. These 23 tasks are the operational activities carried out by the maintenance team which involves processes like isolating the storage units, draining hydrogen, testing & repairing pressure relief valve using inert gas, draining inert gas & refilling hydrogen back in storage unit. These activities have critical interactions like isolating storage unit before draining hydrogen or verifying zero pressure of storage unit before filling inert gas & so on. Such critical interactions lead to emerging risks for example residual gas in the storage unit because of sequence/directional variability in valve operations. While the traditional approaches might detect the residual gas as an error, the root causes may be oversimplified as human error or technical malfunctions. In such a case deploying socio-technical safety barriers like a digital permit to work can prevent sequence/directional variability in the system, i.e, the root cause. Subedi et al. (2025) provides a framework on how to reframe the safety barriers as socio-technical systems. Nevertheless, modeling of complex systems along with socio-technical safety barriers has not been extensively studied.

The SD model, initially published by (Forrester, 1958) is a method to simulate complex systems through interdependent factors, feedback loops, & time delays. It can be exploited to model & understand complex socio-technical systems as the key concept of SD aligns with STS attributes. Feedback loops & system thinking aligns with interdependence of system components, delays & non-linearity concept in SD can signify adaptive & emergent behavior of the system. Nevertheless, SD allows one to develop a systemic digital twin that will not only represent components involved but also the entire interconnected systems. Hence, a SD model of a hydrogen refueling station maintenance procedure can simulate complex interactions along with performance of socio-technical safety barriers, leveraging real time data.

While SD enable the creation of digital twins that capture feedback loops, delays, & non-linear interactions, these models often depend on assumed structures & parameter estimates. Such assumptions can limit their ability to fully represent real world complexity, especially when data are noisy or incomplete. To address this challenge of complex systems, data-driven approaches enable the modeling of the system through discovery of equations directly from observational data. A well-established framework for this task is SINDy (Brunton et al., 2016), which employs symbolic regression to identify the set of governing terms. Notably, SINDy remains effective even when the full state vector is partially unobserved, thereby reducing dependence on unverified theoretical assumptions. The present work focuses on demonstrating the feasibility of using data-driven approaches to quantify SD rather than conducting comparative benchmarking of different methodologies. Integrating SD with SINDy creates a robust framework that combines causal modeling with data-driven discovery to achieve both interpretability & accuracy in representing SD. The accurate representation of SD can then strengthen the evaluation of socio-technical safety barriers deployed within the system.

3. Methodology

This study models the part of maintenance procedure of hydrogen refueling stations; emptying the hydrogen tank for maintenance. The model focuses on assessing the effectiveness of two socio-technical safety barriers: communication & stable zero enforcement reliability to minimize residual gas accumulation caused by system dynamics & operational errors. The stable zero enforcement reliability is presented by two auxiliaries: stable zero enforcement time & stable zero enforcement effectiveness. These barriers aim to counter reinforcing feedback loops in SD model, thereby reducing residual hydrogen. The methodology employs ML-based approaches in two stages: dataset generation & pre-processing, & ML model.

3.1. *Dataset*

3.1.1. *Dataset generation*

The dataset used is generated from a SD model representing the operation involved in maintenance of hydrogen refueling station. The following are the initial conditions & system parameters:

- Initial mass of gaseous hydrogen is 100 kg at 350 bar & 300 K
- Volume of the tank is 4.4 m^3
- Complete natural release of hydrogen occurs at 1839 seconds without any errors.
- Initial residual mass of hydrogen at 1839 seconds is 0.353 kg

Figure 1 illustrates the conceptual structure of the SD model. The model includes the essential feedback loops, barrier interactions, & state variables that govern residual gas accumulation & detection during maintenance. The key variables relevant to this study are communication quality reliability, stable zero enforcement reliability, probability of error generation, residual gas in hydrogen tank & residual gas discovery, pending vent. The intermediate operator actions & minor causal pathways are represented as conceptual auxiliaries to maintain a tractable structure for data generation. The model is built on two explicit assumptions: (i) error generation dynamics follows a simplified probabilistic mechanism influenced by barrier reliability, (ii) safety barriers behave deterministically within each simulation run. These assumptions were necessary to isolate the effect of socio-technical safety barriers. The results should therefore be interpreted strictly within the context of the assumed SD structure, as the synthetic data inherently encode the same modeling assumptions that the SINDy algorithm attempts to identify. The variations in the sparsity threshold, polynomial library, or sample density influences the specific numerical coefficients recovered by SINDy. Nevertheless, across alternative tests conducted during the system identification, the qualitative roles of the barriers remained consistent. This suggests that, under the imposed assumptions, the interaction patterns identified by SINDy are internally consistent. The dataset & pre-processing steps are fully documented to ensure reproducibility of the ML approach and are available at the GitHub repository *link*. Additionally, the ML algorithm used in this study is designed to address scenarios where not all system components are directly measurable, thereby enabling the inference of latent variables within the SD model.

3.1.2. *Pre-processing*

The dataset comprises 243 samples across seven features, derived from an experimental design. Raw simulation data were generated for 27 distinct parameter combinations, corresponding to three discrete levels each for communication reliability, enforcement time, & enforcement effectiveness, evaluated over nine time steps. Each simulation initiates at 1840 seconds, corresponding to the time required to fully evacuate the tank. Table 1 details the dataset features, including their units, corresponding symbols in the SD equations, & data types. During pre-processing, the time column was removed, as the SINDy algorithm requires only the timestep between observations. The remaining features were partitioned into input features, such as residual gas discovery, probability of error generation, & residual gas in the hydrogen tank & control features, consisting of the remaining three features. Additionally, the variable “stable zero enforcement time” was normalized to a [0,1] range to align with the scaling of other input features, thereby mitigating potential model bias due to disparate feature magnitudes.

3.2. *Machine learning model*

3.2.1. *Model setup*

In this work, an ML model based on the SINDy method (Brunton et al., 2016) was implemented to infer the governing equations of the SD. To reflect the discrete-time nature of the available data, the DiscreteSINDy variant of the algorithm was employed. For system identification, the model requires a predefined library of candidate functions from which to construct potential terms in the dynamical equations. A PolynomialLibrary was selected for this purpose, which generates polynomials & interaction terms from input features. The maximum polynomial degree for the candidate functions was constrained to two.

3.2.2. *Training setup*

Two distinct training approaches were implemented. First, a coefficient-focused approach was used to analyze the interpretability of the discov-

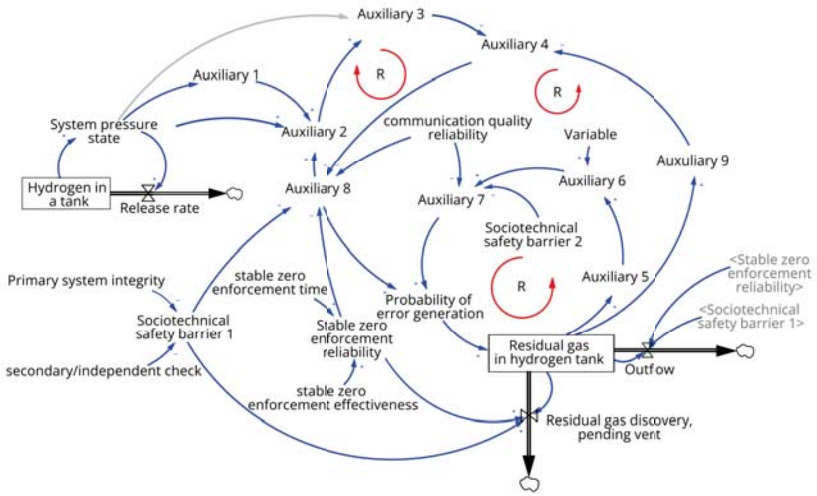

Fig. 1.: Conceptual structure of system dynamics model.

Table 1.: Features & example categories of the dataset

Features	Units	Symbols	Data type
Time	Seconds	k	Integer
Communication quality reliability	Dmnl	u_0	Float
Stable zero enforcement time	Seconds	u_1	Integer
Stable zero enforcement effectiveness	Dmnl	u_2	Float
Residual gas discovery, pending vent	kg	x_0	Float
Probability of error generation	Dmnl	x_1	Float
Residual gas in hydrogen tank	kg	x_2	Float

ered governing equations. For this purpose, the dataset was partitioned into 18 training & 9 testing datasets, approximating a 70/30 split, to assess not just the model's coefficients but also the prediction performance. Second, a prediction-focused approach was adopted to solely assess the model's prediction performance. Given the limited dataset size, bootstrapping (Efron and Tibshirani, 1994) was applied to simulate a larger sample size, enabling the computation of confidence intervals for evaluation metrics. This enhances the statistical reliability of the performance estimates. Both approaches utilized the Sequentially Thresholded Least Squares (STLSQ) optimizer, consistent with the optimizer outlined in Brunton et al. (2016). To promote sparsity, the threshold parameter was set to 0.5 for the coefficient-focused approach & to 0.4 for the prediction-focused approach. Input features were normalized prior to model fitting, while all other hyperparameters remained in their default settings.

3.2.3. *Evaluation*

To evaluate the performance of the identified SD, the coefficient of determination R^2 was computed. Based on Steel and Torrie (1960), the R^2 score indicates the proportion of variance in the observed outcomes that is explained by the model. In this work, it should be interpreted as a measure of short-horizon fit rather than long-term predictive validity. During evaluation, the model iteratively generates a one-step-ahead prediction for each input feature based on the current system state. These predictions are then compared to the corresponding actual values in the subsequent time step according to the evaluation metric.

4. Results & Discussion

4.1. *Coefficient-focused outcomes*

The SINDy method identified discrete equations for residual gas discovery, pending vent (x_0), probability of error generation (x_1), & residual gas in hydrogen tank (x_2) with a good fit $R^2 = 0.910$ as presented in equations 1. The polynomial library with degree two & STLSQ sparsification of threshold = 0.5 balanced the interpretability & fidelity of the operational procedure. The equations generated include the SD with pairwise interactions among the features, thereby enabling quantitative attribution of socio-technical safety barriers on residual gas & probability of error generation.

Equation 1a for residual gas discovery pending vent establishes detection-driven role of the barriers when errors are present. The barrier coupling term: $+0.613\,x_1[k]\,u_0[k] + 0.326\,x_1[k]\,u_1[k] + 0.284\,x_1[k]\,u_2[k]$ indicates that better communication & stronger enforcement increase next step residual gas discovery, pending vent under error prone conditions. This means the socio-technical safety barriers surface latent issues rather than suppressing the discovery signal. The weak damping $-0.091\,x_0[k]^2$ & mitigating cross-terms with residual mass $+-1.656\,x_0[k]\,x_2[k] - 1.897\,x_1[k]\,x_2[k]$, limit persistence when residual gas is present & being addressed. This is because enforcement signals indirectly suppress the probability of error x_1 from equation 1b $-0.444\,x_1[k]\,u_1[k] - 0.427\,x_1[k]\,u_2[k]$. Hence lower future probability of error will then decay the pending vent status faster. This results in pending vent issue goes away faster hence resolving sooner through discovery. This aligns with intent of socio-technical barriers: communication reliability will enhance observability & enforcement enhances corrective control.

The probability of error generation, Equation 1b, shows how the barriers stabilize the error dynamics. The auto-regressive coefficient $+1.700\,x_1[k]$ & positive quadratic $+0.684\,x_1[k]^2$ indicates reinforcing loops as in system dynamic model. The effect of barriers are all stabilizing & trio of barriers $-0.349\,x_1[k]\,u_0[k] - 0.444\,x_1[k]\,u_1[k] - 0.427\,x_1[k]\,u_2[k]$ jointly suppress the probability of error generation.

The equation 1c for residual gas in hydrogen tank indicates that residual mass declines once it is discovered & coordinated action is taken. The term $-0.387\,x_0[k]$ shows that discovery of residual gas precedes residual gas reduction at the next step, & the communication coupled term $-0.760\,x_0[k]\,u_0[k]$ further strengthen this effect. This is consistent with better communication & coordination once the situation is known. Small positive couplings $+0.046\,x_2[k]\,u_1[k]$ & $+0.026\,x_2[k]\,u_2[k]$ suggest that strict enforcement can, in some contexts, transiently slow the clearance of residuals, e.g., due to checks or pauses, while a small $+0.045\,x_0[k]\,u_2[k]$ indicates occasional overhead when corrective steps are enforced during discovery. In summary, communication plays the *direct* role in accelerating mass decay after discovery, whereas enforcement contributes *indirectly* by suppressing error persistence & supporting the overall resolution of the residual gas discovery, pending vent.

In nutshell, several coupling coefficients of barriers produced mixed signs across equations, underscoring the context-dependent role of barriers in socio-technical systems. For example, enforcement can surfaces deviations before ultimately reducing them. This behavior is consistent with the paper's objective to move beyond static fixed efficiencies approach) towards dynamic system based interactions. This work enables marginal & conditional measures of barrier effectiveness. With the equations, it open possibilities to simulate what-if scenarios & one can construct trade off frontiers (residual mass vs. time-to-safe-state vs. error probability), thus converting the equations into operational guidance for barrier configuration.

The developed SINDy-based model achieves high in sample fit of $R^2 = 0.910$ & yields equations that are interpretable in terms of barrier interactions. However, rigorous validation is still required to substantiate application of the model.

$$\begin{aligned}x_0[k+1] = {} & -0.665 + 0.697\,x_1[k] - 0.091\,x_0[k]^2 + -1.656\,x_0[k]\,x_2[k] - 1.897\,x_1[k]\,x_2[k] + 0.613\,x_1[k]\,u_0[k] \\ & + 0.326\,x_1[k]\,u_1[k] + 0.284\,x_1[k]\,u_2[k] + 2.520\,x_2[k]^2 \end{aligned} \tag{1a}$$

$$\begin{aligned}x_1[k+1] = {} & 0.182 + 1.700\,x_1[k] - 0.654\,x_2[k] - 2.656\,x_0[k]^2 + 13.382\,x_0[k]\,x_1[k] - 10.489\,x_0[k]\,x_2[k] \\ & + 0.684\,x_1[k]^2 - 11.552\,x_1[k]\,x_2[k] - 0.349\,x_1[k]\,u_0[k] - 0.444\,x_1[k]\,u_1[k] - 0.427\,x_1[k]\,u_2[k] \\ & + 10.775\,x_2[k]^2 \end{aligned} \tag{1b}$$

$$\begin{aligned}x_2[k+1] = {} & 0.153 - 0.387\,x_0[k] + 0.919\,x_2[k] - 0.760\,x_0[k]\,u_0[k] + 0.045\,x_0[k]\,u_2[k] + 0.046\,x_2[k]\,u_1[k] \\ & + 0.026\,x_2[k]\,u_2[k] \end{aligned} \tag{1c}$$

Importantly, despite the limited data set (Cartesian grid over three barriers with short time horizons) & partial observability of the underlying system, the SINDy method was able to recover a compact representation of dynamics only a subset of the twin variables of SD served as input to identification, yet the learned equations remained coherent with the hypothesized detect then correct mechanism of socio-technical barriers.

4.2. *Prediction-focused outcomes*

When the SINDy method was applied with an emphasis on prediction performance rather than coefficient interpretability, the resulting model demonstrated significantly improved accuracy, achieving an average $R^2 = 0.965$ across 200 bootstrapped subsets. As shown in Figure 2, the 95% confidence interval for the R^2 score lies between $[0.938, 0.979]$, underscoring robust short-horizon predictive performance under the assumed data-generating process. This improvement can be attributed, in part, to the reduction of the sparsity threshold from 0.5 to 0.4, which permitted less sparse & potentially more precise governing equations. Consequently, the prediction-focused models exhibited both higher accuracy & greater functional complexity compared to the coefficient-focused approach. Analysis of randomly selected models from the ensemble confirmed that the discovered governing equations consistently retained all control features. This indicates that each safety barrier remains coupled within the SD, even when the modeling objective prioritizes predictive performance over the interpretability of individual coefficients.

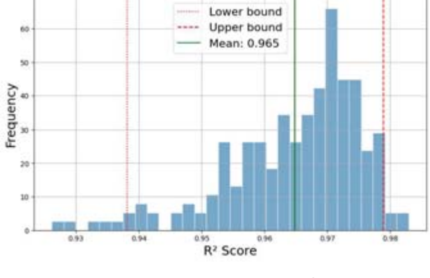

Fig. 2.: Histogram of the R^2 score.

While this second SINDy-based model achieved a higher R^2 score than the first, its interpretability was reduced due to the increased number of functions in the equations, making explicit dependency analysis more challenging. This result illustrates a trade-off inherent to data-driven modeling: a robust, high performance predictive model can be constructed at the expense of interpretability. Depending on the application, such a trade-off may be acceptable or even desirable. In this work, the SINDy framework for socio-technical systems successfully demonstrated that both interpretable models & high-accuracy predictive models can be derived from the same dataset, offering flexibility depending on the analytical priorities.

5. Conclusion

This study demonstrated a quantitative modeling approach to represent and analyze the dynamic influence of socio-technical safety barriers during hydrogen refueling station maintenance operations by exploiting the SD twin for data generation, & the SINDy algorithm for system identification & model performance evaluation. The use of discrete polynomial library with SINDy algorithm yielded compact governing equations that captured socio-technical attributes of the safety barriers. The use of two configurations: coefficient focused model & prediction focused model established that it is feasible to learn complex dynamics while maintaining interpretation & high quality prediction from limited & partially observed data. The identified system dynamics focused on coefficient established a clear division of barrier performances. Communication primarily improves detection & coordination. This would help identify residual gas when errors exist & accelerate residual gas discovery for venting out. Enforcement time & effectiveness factor acts as detection & stabilization by potentially increasing discovery of residual gas by surfacing deviations, while damping the persistence of probability of error over subsequent steps. This subsequently resolves the apparent tension between increased residual gas discovery & increased safety. The barriers briefly increase the probability of error because they make error visible, yet they reduce the mechanism that sustain it. The second prediction focused model achieved higher accuracy with balance of functional complexity. Notably, both models retained barrier couplings indicating barriers are structurally relevant, & allowing one to choose an interpretable or predictive model depending on the need.

The study has some limitations that point to immediate next steps. The identified models are not unique representations of the system dynamics, and their applicability in real operational settings remains unverified. To improve generalization, future work should use larger datasets & incorporate additional input & control features that reflect real hydrogen system operations. Performance & interpretability could be enhanced by designing a custom function library informed by system dynamics, FRAM, & domain expertise. Finally, applying the approach to additional maintenance procedures & safety barriers would help establish its robustness and readiness for practical use in hydrogen applications.

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