Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale, Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

Integrating Thermodynamic Simulation and Surrogate Modeling to Find Optimal Drive Cycle Strategies for Hydrogen-Powered Trucks

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ABSTRACT

Hydrogen-powered heavy-duty trucks have a high potential to significantly reduce CO_2 emissions in the transportation sector. Therefore, efficient hydrogen storage onboard vehicles is a key enabler for sustainable transportation, as achieving high storage densities and extended driving ranges is essential for the competitiveness of hydrogen-powered trucks. Cryo-compressed hydrogen (CcH_2), stored at cryogenic temperatures and high pressures, emerges as a promising solution. This study presents a comprehensive dynamic thermodynamic model that is capable of simulating the tank system across all operating conditions and, therefore, enables thermodynamic analysis of drive cycles. The core of the model is a differential-algebraic equation system that describes the thermodynamic state of the hydrogen in the tank. Additionally, surrogate models based on artificial neural networks are applied to efficiently describe quasi-steady-state heat exchangers integrated into the tank system. Several use cases are explored to demonstrate the model's ability to simulate the thermodynamic behavior and to find optimal operating strategies. The optimal hydrogen density, when to stop driving and refuel the tank to maximize overall driving ranges, is investigated both in ideal and real operation, taking into account the limited availability of refueling stations in early market applications. Further, driving range and venting losses are considered for longer periods of dormancy. These results provide insights into how operational strategies can be tailored to maximize driving range, minimize hydrogen losses, and improve overall system efficiency, ultimately supporting the adoption of hydrogen in long-haul transportation.

Keywords: Hydrogen, Dynamic Modeling, Surrogate Model, Process Operations, Matlab

INTRODUCTION

To reduce CO_2 emissions in transportation, hydrogen-powered heavy-duty trucks are a promising solution. Thereby, cryo-compressed hydrogen (CcH_2), stored at cryogenic temperatures and high pressures, is an efficient way for onboard hydrogen storage, as it achieves the highest storage densities [1]. In the CryoTRUCK project, funded by the German Federal Ministry of Digital and Transport (BMDV), such a CcH_2 storage is being developed. For optimal utilization of the stored hydrogen, good knowledge of the thermodynamic processes within the tank is essential. Thus, in previous works, thermodynamic models and computational fluid dynamics (CFD) analyses studying the heat exchangers of the tank system have been introduced [1-5]. This study applies and combines the thermodynamic models of the tank system to analyze and investigate optimal vehicle operation.

Therefore, surrogate models based on artificial neural networks (ANNs) are used to efficiently simulate the heat exchangers integrated into the system, enhancing simulation speed and reducing model complexity. This model reduction allows the export of the tank model in a compact way for integration into large vehicle models or even for onboard simulations. Several use cases are explored in this study, focusing on optimal operation to maximize driving range or avoid hydrogen losses.

METHODOLOGY

The applied model consists of a dynamic thermodynamic tank model and surrogate component models of two heat exchangers that will be discussed hereafter.

Thermodynamic Tank Model

The considered CcH_2 tank is depicted in Figure 1. It consists of an aluminum liner wrapped in carbon fiber and insulated by vacuum and multi-layer insulation. Two heat exchangers are included in the system: an inner (iHEX) and an outer (oHEX) heat exchanger. The latter one heats up the cryogenic hydrogen that is discharged from the tank (mass flow rate $\dot{M}_{\mathrm{disch}}$) before the warm hydrogen is fed to the truck's fuel cell (FC). The iHEX is used to control the pressure in the tank by heating the tank (heat flow $\dot{Q}_{\mathrm{disch}}$). Therefore, hydrogen that has already been heated up in the oHEX is redirected via a three-way valve to the iHEX. After passing the iHEX, the hydrogen flows through the oHEX once more towards the FC.

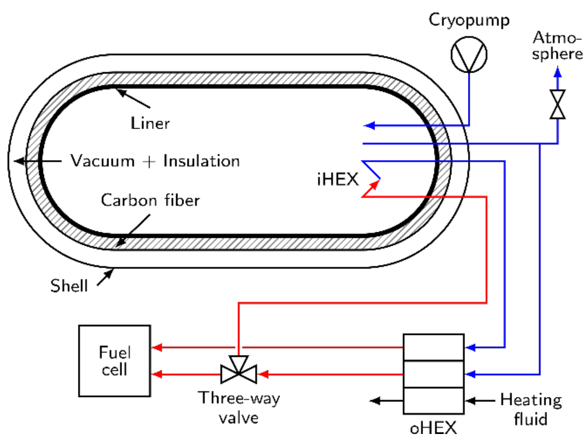


Figure 1. CcH2-Tank [2]

Three operating scenarios are considered in this study: discharge (or driving), refueling, and dormancy. In this study, it is assumed that in the refueling scenario, CcH_2 is always refueled with a constant mass flow rate $\dot{M}_{\mathrm{fuel}} = 60\ \mathrm{g}/s$ as described in [2]. Further, when the truck is parked for a long time, the pressure may rise above the venting pressure $p_{\mathrm{vent}} = 450\ \mathrm{bar}$ due to heat inleak from the ambiance (heat flow $\dot{Q}_{\mathrm{amb}}$), which requires venting hydrogen with the mass flow rate $\dot{M}_{\mathrm{vent}}$ to maintain the pressure p_{vent}. It is assumed that exactly the amount required to maintain the pressure is vented.

When simulating a discharge process, a constant mass flow rate of $\dot{M}_{\mathrm{disch}} = 1\ \mathrm{g}/s$ is considered. As shown in previous work [1,2], the temperature and pressure in the tank decrease during driving. When the minimum pressure $p_{\mathrm{min}} = 15\ \mathrm{bar}$ required by the FC system is reached, the iHEX is turned on. [1] and [2] assume that the iHEX delivers exactly the heat required for maintaining the pressure p_{min}, which will be referred to as *ideal iHEX*. In this study, it is assumed that the three-way valve in Figure 1 acts as on-off control, meaning that either all discharged hydrogen is passed through the iHEX or none. When the iHEX is on, the temperature and pressure in the tank rise. As soon as an upper threshold is reached, the iHEX is shut off again. Here, the upper threshold is set to 35 bar. The heat flow generated by the iHEX is calculated from surrogate models that will be discussed in the next section. This setup is hereafter referred to as *real iHEX*.

Thus, the CcH_2 tank is characterized by the mass and energy balance in Equation (1) and (2). For the sake of simplicity, no index is used for all variables describing the hydrogen within the tank.

$$\frac{\mathrm{d}M}{\mathrm{d}t} = \dot{M}_{\mathrm{fuel}} - \dot{M}_{\mathrm{disch}} - \dot{M}_{\mathrm{vent}} \tag{1}$$

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \dot{M}_{\mathrm{fuel}} \cdot h_{\mathrm{fuel}} - \dot{M}_{\mathrm{disch}} \cdot h - \dot{M}_{\mathrm{vent}} \cdot h + \dot{Q}_{\mathrm{amb}} + \dot{Q}_{\mathrm{disch}} \tag{2}$$

As it is assumed that the hydrogen is ideally mixed, the hydrogen taken from the tank has the same temperature and pressure and, therefore, specific enthalpy h as the hydrogen in the tank. The specific enthalpy h_{fuel} of the refueled hydrogen results from an isentropic compression from the refueling station pressure to the tank pressure p with the efficiency $\eta_{\mathrm{pump}} = 0.78$ until the fill pressure $p_{\mathrm{fill}} = 400\ \mathrm{bar}$ is reached [2]. Further, only the hydrogen as well as the solid aluminum and carbon fiber parts are considered, while other solid components of the tank are neglected. As the solids are in good thermal contact with the hydrogen, a uniform temperature is assumed [1,2]. Based on the balances and several algebraic equations, a differential-algebraic equation system is defined in [1] and [2], describing the thermodynamic state of the hydrogen in the tank for all operation modes. All parameters used for this study are taken from [2].

Surrogate Component Models

Within the CryoTRUCK project, rigorous component models of the two heat exchangers in the tank are being developed, based on thermodynamic correlations and CFD simulations [4,5]. Combining these models with the dynamic thermodynamic tank model would highly increase calculation time and model complexity. However, using the model for real drive cycle optimizations, integration into large vehicle models, or usage onboard the truck for driver assistance systems and tank state monitoring requires real-time calculations and low complexity. Thus, surrogate models of the heat exchangers are generated and integrated into the tank model. It is assumed that both heat exchangers are in a quasi-steady state in relation to the dynamics of the CcH_2 tank.

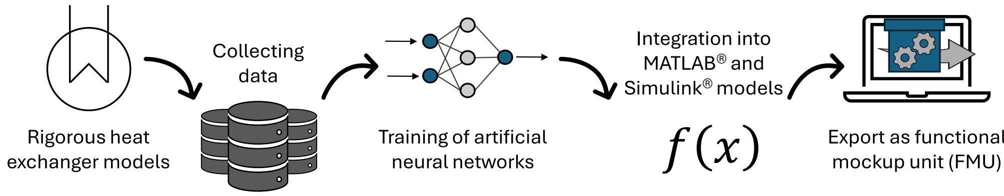


Figure 2. Workflow of building the surrogate models.

The workflow of generating these surrogate models is shown in Figure 2. The rigorous heat exchanger models are used to collect datasets of input-output relations for the steady-state heat exchanger characteristics. The inputs are chosen across the operation range using Latin hypercube sampling [6]. The data is used to train, validate, and test ANNs, which take all inputs of the respective rigorous models and return the hydrogen state at the outlet of the heat exchanger and the transferred heat flows. When the ANNs are inserted into the MATLAB® system model, the resulting reduced model includes only two differential equations and accurately represents the overall system while having low model complexity. Additionally, by integrating the ANNs into a Simulink® tank model and exporting it as a functional mockup unit (FMU), the model can be included in other simulation platforms and possibly run onboard a truck.

RESULTS

This section investigates drive cycles with the ideal and real heat exchanger models. Further, two case studies of typical operating strategy problems are conducted.

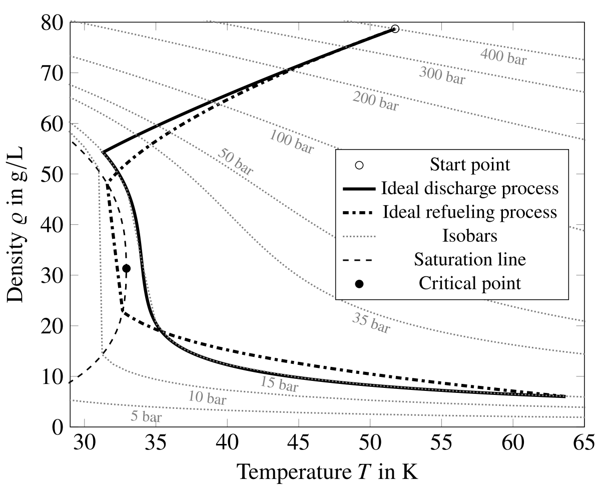


Figure 3. Drive cycle with ideal iHEX

Figure 3 shows an ideal cycle of discharge and refueling with the ideal iHEX within a (T, ϱ)-diagram. At the beginning of the discharge, temperature and pressure decrease. When reaching p_{min}, the iHEX is switched on and delivers exactly the heat flow required to follow the p_{min}-isobar. As soon as a minimum density, also called stop density ϱ_{stop}, is reached, the truck is stopped and refueled up to p_{fill}, ending up at the same thermodynamic state as at the beginning of the idealized cycle.

The real discharge process, deploying the real iHEX simulated with the surrogate models and the on-off control, is depicted in Figure 5(a) alongside the ideal process. Generally, the real process follows the ideal one, however, due to the on-off control, a zigzag pattern is visible. When p_{min} is reached and the iHEX is turned on, more heat than required is transferred. Thus, temperature and pressure rise. When the iHEX is shut off at 35 bar, temperature and pressure fall back to the path of the ideal process. At the end of the discharge, much more heat is required to keep the pressure, and the intervals of heating become larger. However, the heating intervals highly depend on the mass flow rate and the starting conditions.

These findings are relevant when considering the influence of ϱ_{stop} on the usable density $\Delta\varrho_{\mathrm{use}}$ and the fill density ϱ_{fill}, which are plotted over the stop density in Figure 4 for the ideal process, assuming that refueling is possible at any time [2]. The fill density is defined as the density that results from refueling up to p_{fill}, starting from the thermodynamic state at the end of the discharge defined by ϱ_{stop}. The usable density $\Delta\varrho_{\mathrm{use}} = \varrho_{\mathrm{fill}} - \varrho_{\mathrm{stop}}$ relates the current stop density to the subsequent fill density and, thus, to the potential driving range of the next drive cycle.

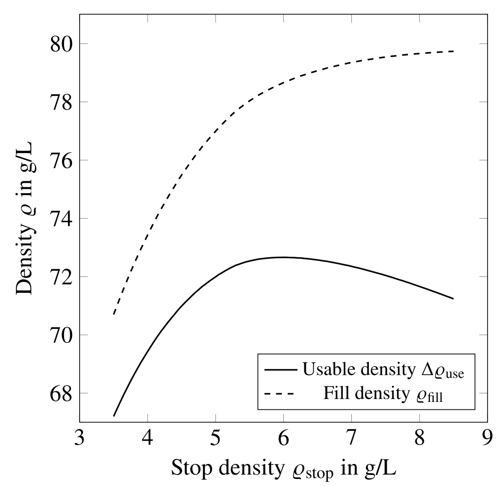
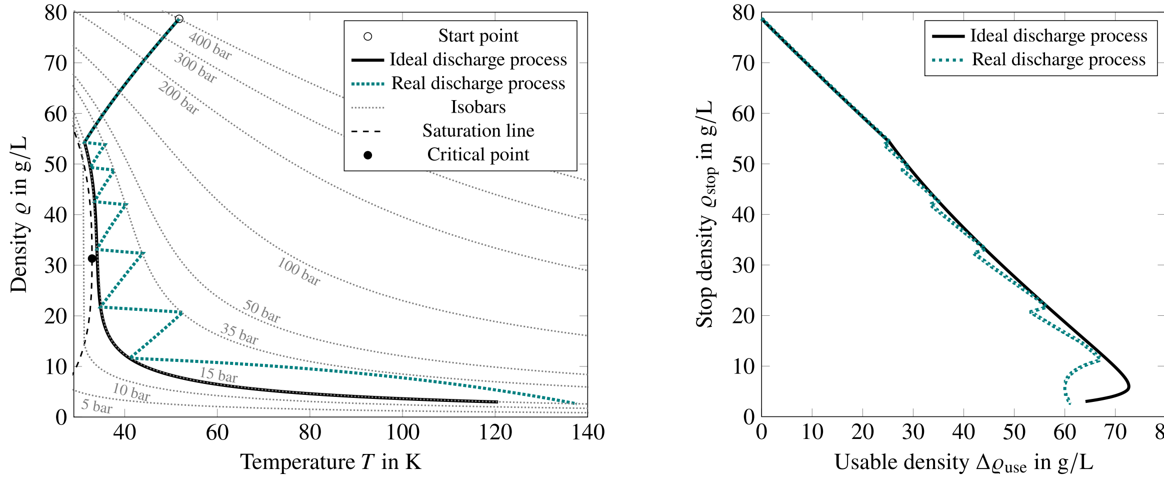


Figure 4. Usable and fill density as a function of the stop density



(a) Discharge process (b) Usable density

Figure 5. Discharge process and corresponding usable densities for refueling anytime during the discharge

The fill density highly depends on ϱ_{stop}, as at the end of the discharge, the temperature rises fast when the p_{min}-isobar slope becomes small (see Figure 3). For the following refueling process, however, low temperatures in the tank are preferable to achieve higher storage densities. Consequently, the fill density increases in Figure 4 for higher stop densities. Since stopping too early would not exploit the capacity of the tank, the usable density has a clear maximum. Thus, for the ideal process, an optimal stop density, at which it is best to stop and refuel for the maximum driving range, can be found by optimizing $\Delta\varrho_{\text{use}}$. Therefore, the MATLAB® function `fminbnd` is applied to maximize $\Delta\varrho_{\text{use}} = f(\varrho_{\text{stop}})$. The underlying objective function calculates $\Delta\varrho_{\text{use}}$ by simulating a refueling process, starting from the thermodynamic tank state defined by ϱ_{stop} and p_{min}. The resulting optimal stop density is $\varrho_{\text{stop}}^{\text{ideal}} = 6.025\,\text{g/L}$, which corresponds to a fill state of $\varrho_{\text{fill}} = 78.69\,\text{g/L}$, $T_{\text{fill}} = 51.75\,\text{K}$, and $p_{\text{fill}} = 400\,\text{bar}$. This is used as starting point for all remaining simulations.

When, instead, the real iHEX, including the on-off control, is considered, a different behavior is observed. Figure 5(b) shows the usable density that would be achieved when the truck is stopped and refueled at any time during the ideal and real discharge processes in Figure 5(a). Thereby, the thermodynamic state corresponding to each stop density in Figure 5(b) equals a state in Figure 5(a). The results of the ideal iHEX process are in accordance with the course in Figure 4 and show an optimum at $\varrho_{\text{stop}} = 6.025\,\text{g/L}$. The usable densities simulated with the real iHEX, however, are highly influenced by the peaks due to the on-off iHEX control. Whenever the iHEX is on and the temperature in the tank is high, refueling would be less efficient. Thus, the usable density is best when refueling just before the iHEX is turned on again. At the theoretical optimal stop density, the real process course for the considered starting conditions and mass flow rate is at the peak of a heating period, which is most unfavorable for refueling. Consequently, the real iHEX process would have roughly 5 g/L less maximal usable density compared to the ideal case. When still stopping at the theoretical optimal stop density, 12 g/L of maximal usable density is lost.

While this approach allows calculating optimal stop densities for the real system and could, thus, be used to recommend when to refuel, an even better approach to maximize the usable density would be to alter the iHEX control before refueling. When the truck operator provides the tank system with knowledge of the next refueling point, the iHEX could be turned off to ensure low temperature and pressure when refueling takes place.

Case Study 1: Refueling Station Scarcity

In this section, the ideal and real discharge processes are investigated, considering that during early market entry, only limited hydrogen refueling stations exist. Two cases are defined: refueling stations are located (a) every 100 km, or (b) every 50 km. It is assumed that a truck has two tanks as defined in [2] and that a hydrogen truck consumes roughly 7 kg per 100 km [7]. Figure 6 highlights all options for refueling during the discharge process in a (T, ϱ)-diagram. The resulting usable densities at all refueling stations are depicted in Figure 7(a) and Figure 7(b) for the cases where refueling stations are located every 100 km or every 50 km. Most deviations between the ideal and real iHEX operation occur after long driving ranges because, for the considered mass flow rate and starting conditions, the drive cycle ends with a long period of heating of the real iHEX, which is non-ideal for the subsequent refueling.

In the 100 km case, the last two fuel stations lead to almost the same usable density in the real discharge process, even though the last tank stop is located at the peak of the last heating period. The non-ideal refueling conditions at the last stop are balanced out by refueling too early at the second last option, not exploiting the usable density.

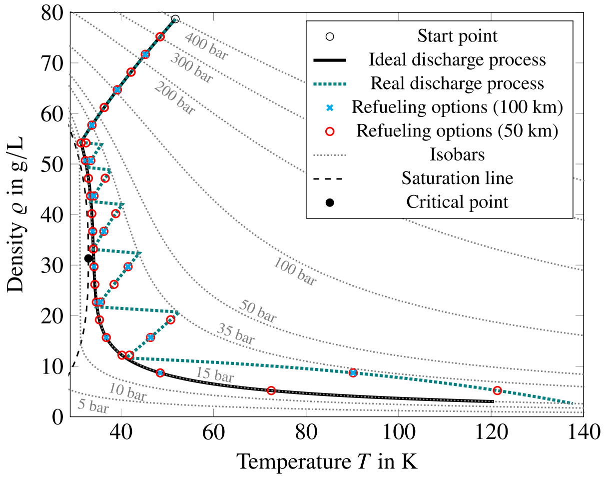


Figure 6. Discharge process with markers for refueling stations which are located every 100 or 50 km.

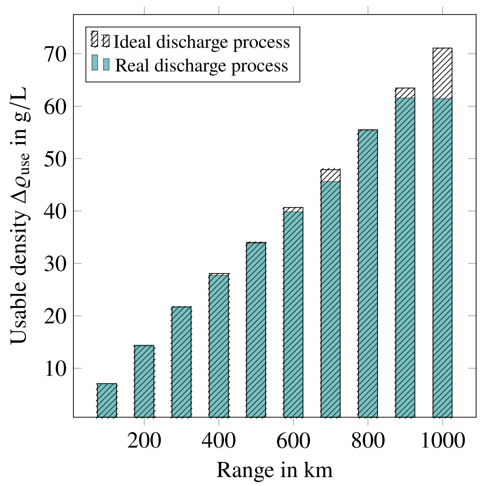
In the 50 km case, the third last stop option is the preferred one. Here, the refueling stop happens just before the next heating period starts. Thus, almost the usable density of the ideal iHEX process is reached. Stopping at the last option, however, would even be worse than the fourth last stop in terms of usable density.

Case Study 2: Long Dormancies

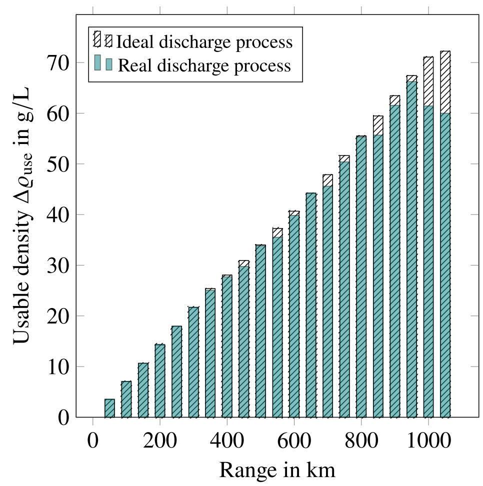
In a second study, the effect of longer dormancies, e.g., when the truck is parked for the weekend, on the drive cycle operation is investigated. First, the truck is driving until the stop density $\varrho_{\mathrm{stop}} = 6.025$ g/L is reached. Then, it can either be refueled before being parked for the weekend for 62 h (A), or afterward, before starting the next drive after the weekend (B). Figure 7(a) shows both options in a (T, ϱ)-diagram.

In both cases, temperature and pressure rise during dormancy due to heat leaking into the tank. When, in (A), the pressure reaches the venting pressure p_{vent} after more than 36 h, hydrogen is vented. Further, since the stop density is reached during a heating period, the refueling process is not ideal. Nevertheless, at the end of the cycle, the tank in (A) is fuller than in (B), where the empty truck is parked for the weekend and refueled after the dormancy, which prevents venting. In (B), the refueling conditions are worse than in (A) as the tank has warmed up during dormancy. Additionally, the temperature increases faster in an empty tank. Thus, even though in (A) 1.27 g/L of fill density is lost due to venting, a 4.06 g/L higher fill density is achieved. With a consumption of 7 kg per 100km, this translates to roughly 30 km extended range, enabling higher route flexibility and less refueling stops. However, as venting also means economic loss, an economically optimal operation can only be determined if all economic parameters are known.

For longer dormancy, the difference between the endpoints of (A) and (B) becomes smaller, and eventually, there is a turnover point. As it is assumed that in (B) the truck starts driving right after refueling, it could be filled, as compared to (A), to the venting pressure p_{vent}. Considering this procedure, the turnover point is calculated by minimizing the difference in storage density at the end of (A) and (B) with `fminbnd`. Figure 7(b) shows the drive cycle with a dormancy of the calculated turnover point (27.5 days). At this point, 19.4 g/L are vented for case (A). Consequently, depending on whether venting should be prevented or the driving range maximized, an operation strategy can be chosen.

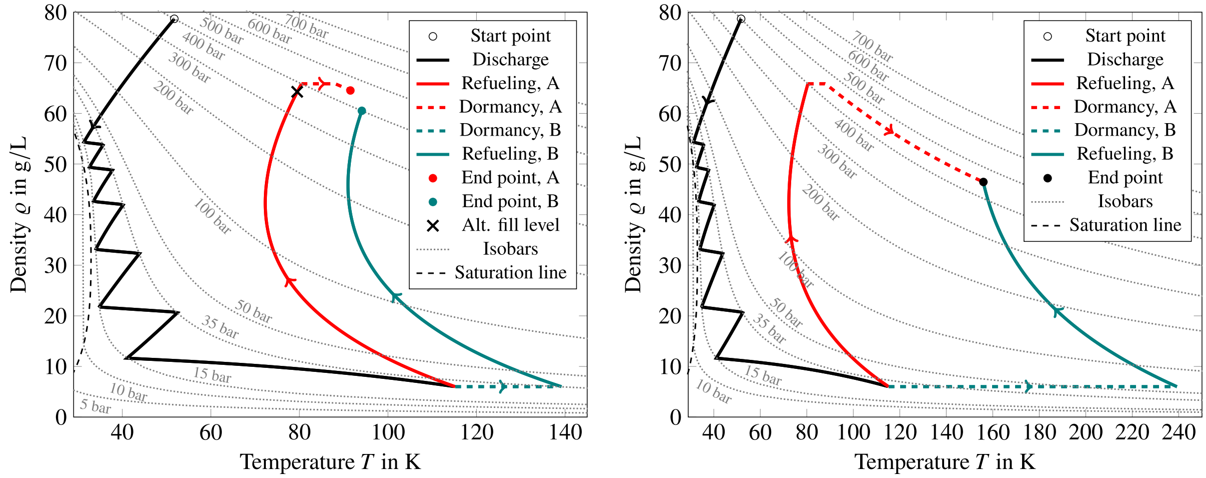


(a) Refueling stations located every 100 km



(b) Refueling stations located every 50 km

Figure 7. Usable density for limited availability of refueling stations.



(a) Drive cycle with 62 h dormancy (b) Drive cycle at turnover point (27.5 days)

Figure 8. Drive cycles of real iHEX consisting of (A) discharge, refueling, and dormancy, and (B) discharge, dormancy, and refueling.

Alternatively, by refueling slightly less than the fill pressure, venting can be fully avoided while still ensuring high fill density. For the 62 h dormancy, this could be achieved by filling to 369.2 bar instead of 400 bar, resulting in a fill density of 64.27 g/L slightly below the final density of case (A) (64.58 g/L). The alternative fill density is marked in Figure 7(a).

CONCLUSION

The presented study combines a dynamic thermodynamic model of a CcH_2 tank for trucks with surrogate quasi-steady-state heat exchanger models based on ANNs. Therefore, this model allows for fast and low-complexity simulations. The resulting system model is used for several case studies, demonstrating the influence of driving strategies on driving ranges and boil-off losses.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the financial support of the joint project "CryoTRUCK" by the German Federal Ministry of Digital and Transport (BMDV, FKZ 03B10411E) and the project supervision by the project management organization Projektträger Jülich (PtJ).

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