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COMSOL/Simulink-Coupling for Optimization of Sorption Heat Storage in Residential Buildings

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Abstract

In this work, a spatially resolved Computational Fluid Dynamics (CFD) model of a closed sorption heat storage reactor employing a zeolite-water sorption pair was developed in COMSOL Multiphysics®. To assess its performance under dynamic boundary conditions in residential buildings, the validated reactor model was integrated into a building energy system model using COMSOL LiveLink™ for Simulink. Building energy components in Simulink were either imported from the CARNOT Toolbox library or developed directly in MATLAB/Simulink. In this coupled setup, the heat transfer fluid (HTF) inlet temperature and mass flow rate, calculated within Simulink, were dynamically transferred to COMSOL as time-dependent boundary conditions. COMSOL then performed transient CFD simulations of the sorption storage unit to resolve coupled heat and mass transfer phenomena. The outlet temperature of HTF and the corresponding useful thermal power were subsequently exported back to Simulink, where they were incorporated into the building energy model for control strategy implementation and determining the thermal energy flow distribution to downstream system components. This co-simulation approach combines the accuracy of physics-based reactor modeling with the flexibility of system-level building simulations, enabling a more realistic assessment of thermochemical energy storage integration. The study demonstrates the feasibility and advantages of this modeling strategy and presents results on the seasonal performance of the coupled system, highlighting the potential of sorption-based storage for enhancing renewable energy utilization in buildings.

Keywords: Sorption Heat Storage, Computational Fluid Dynamics, Building Simulation, FMU, Zeolite

Introduction

Sorption heat storage systems are attracting growing interest due to their high energy density and loss-free heat storage capability, making them a promising solution for storing surplus solar energy in summer for use in winter in residential buildings. Several previously developed prototypes have revealed the high potential of sorption storage systems for seasonal thermal storage; however, these systems are still in the research and development stage. Computational Fluid Dynamics (CFD) simulations can be used to obtain a comprehensive understanding of the complex processes in these systems and to represent them with high temporal and spatial resolution. This makes it possible to adjust the system design and reaction control in a targeted manner to achieve an optimum performance. On the other hand, building simulations are necessary to evaluate the performance of such a system under different boundary conditions and in different locations. In the absence of validated pre-existing models within building simulation environments such as Simulink, the use of an experimentally validated COMSOL Multiphysics® model provides a valuable means to evaluate system performance under realistic operating conditions when integrated with other building energy components. CFD-based models offer high spatial and temporal resolution, enabling accurate prediction of outlet temperatures and output power. Coupling these models establishes a comprehensive framework for analysis and optimization. A validated numerical model of a Zeolite 13X-based sorption storage system was developed in [1]. They emphasize that minimizing system losses requires efficient control and conclude that thermal energy storage systems must be coupled with a numerical building model and associated control strategies to properly evaluate their impact on energy demand. Different building simulation methods are available to study the effect of storage systems on buildings, including software such as TRNSYS, MATLAB, EnergyPlus, and EES, among others. In [2], a building model developed in TRNSYS was coupled with a MATLAB model of a Zeolite 13X reactor and a Compound Parabolic Collector (CPC) to study sorption energy storage under transient conditions. The analysis examined charging and discharging processes, focusing on solar radiation, air mass flow rate, CPC configuration, inlet air moisture, and initial water uptake, including their coupling effects. The model was validated against experimental data, and operating conditions achieving 48.2% charging efficiency and 49% discharging efficiency. In [3], the impact of three European climates (Paris, Munich, Stockholm) on a solar-driven seasonal sorption system for domestic hot water and space heating was evaluated. The system employed LiCl in a silica gel matrix with water as the working fluid. The building model was implemented in OpenStudio with heating demand simulated via EnergyPlus. Python-based numerical models and performance maps were used to assess subsystem behavior under rule-based optimal control. The results showed that solar-driven sorption storage is feasible for residential heating in these climates.

Most studies use TRNSYS or Energy Plus, focusing on chemisorption or composite sorbents [2], [4]. Few works have implemented full building-integrated zeolite physical adsorption models in MATLAB/CARNOT [5]. These approaches either lack the fine physical detail for the reactor or flexibility for the building side. The novelty of the presented work lies in bridging this gap by coupling a high-fidelity COMSOL reactor model with a flexible Simulink/CARNOT building model. The COMSOL model captures reactor-level physics (mass transfer, adsorption kinetics, geometry-dependent effects) with higher fidelity than simplified models. The CARNOT toolbox in Simulink provides ready-to-use building models, HVAC systems, and renewable components, allowing realistic building integration under different climates, load profiles, and control strategies. This hybrid approach combines physical accuracy at the reactor scale with system-level flexibility at the building scale, enabling comprehensive scenario studies.

Physical Model of the Sorption Reactor

In this study, the adsorption and desorption processes of the zeolite/water pair in closed sorption thermal energy storage (STES) system have been studied numerically. In the studied system, during desorption, saturated zeolite in the reactor is dried by the hot heat transfer fluid (HTF), flowing through the heat exchanger, and energy is stored in the zeolite due to the reaction between the zeolite and water. As a result of this process, the water molecules are released from the zeolite in the gaseous state and condensed to the liquid state in the condenser. This reduces the amount of water in the zeolite, and the heat is stored. The process of adsorption begins with the evaporation of water in the evaporator, placed at the bottom of the reactor. The water vapor flows into the reactor and is adsorbed in the pores of dry zeolite. The released energy from this reaction is extracted by the HTF flow. Figure 1 shows the geometry of the STES system, which is composed of finned tubes with adsorbent material packed between the fins. The geometrical dimensions of a single finned-tube unit used in this work are listed in Table 1. In the modeled reactor, 100 such tubes are assembled, resulting in a total storage volume of 0.6 m³.

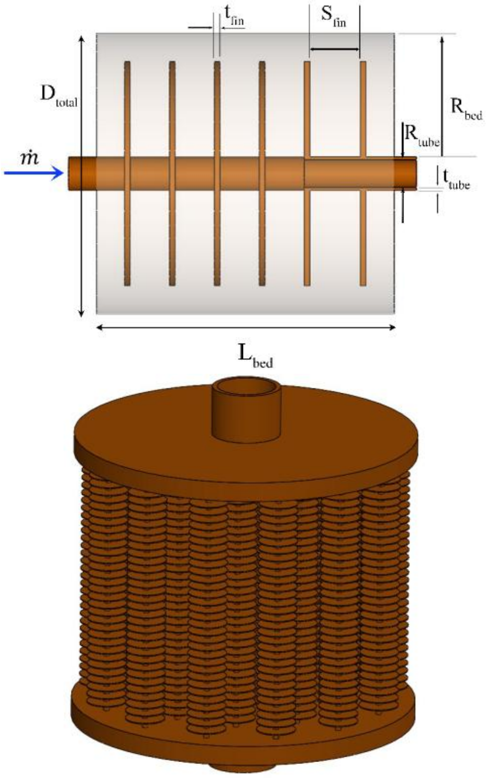

Figure 1. Schematic showing (a) a finned tube unit and (b) the sorption storage reactor.

Table 1. Key geometric parameters

Parameter	Value	Unit	Description
L_{bed}	0.33	m	Bed length
R_{bed}	0.05	m	Bed radius
R_{tube}	0.025	m	Tube Inner Radius
t_{tbue}	0.001	m	Tube thickness
S_{fin}	0.03	m	Distance between adjacent fins
L_{fin}	0.03	m	Fin length
t_{fin}	0.004	m	Fin thickness
N_{fin}	8	-	Number of fins

Governing Equations of the Sorption Process

The adsorbed loading X is determined using the Linear Driving Force (LDF) approach [6]

$$\frac{\partial X}{\partial t} = k_{LDF}[X^* - X] \qquad (1)$$

Here, X^* denotes the equilibrium adsorption capacity, while X represents the instantaneous amount of adsorbed water. The mass transfer coefficient k_{LDF} is defined as:

$$k_{LDF} = \frac{15}{r_p^2} D_{ref} \exp\left(-\frac{E_a}{RT}\right) \tag{2}$$

where r_p is the radius of the zeolite particles, D_{ref} is the reference diffusivity, and E_a is the characteristic energy. Dubinin–Astakhov (DA) theory is used for calculating the equilibrium water uptake [7]:

$$X^* = X_0 \exp\left(-B\left(\frac{T}{T_{sat}} - 1\right)^n\right) \tag{3}$$

Where X_0 represents the maximum adsorption capacity, and B and n are fitting parameters specific to the zeolite–water pair. The mass balance governing the transport of the adsorbed phase can then be expressed as [7]

$$\varepsilon_{eff} \frac{\partial T_s}{\partial t} - D_{eff} \nabla^2 c + \nabla(c.u) = -\frac{(1-\varepsilon_{eff})\rho_s}{M_w} \frac{\partial X}{\partial t} \tag{4}$$

where c is the water vapor concentration, D_{eff} is the effective diffusion coefficient, ρ_s is the density of the adsorbent, M_w is the molar mass of water vapor. The vapor velocity field in the sorbent bed is solved using the Darcy model. For solving energy equations, three different regions are considered: the adsorbent bed, the HTF, and the HTF tube. The energy equations for the adsorbent bed can be written as [7]:

$$\begin{aligned}&(\varepsilon_{eff}\rho_f C_f + (1-\varepsilon_{eff})\rho_s C_s + (1-\varepsilon_{eff})\rho_s C_l X)\frac{\partial T}{\partial t}\\ &+\rho_f C_{p,f} u.\nabla T - k_{eff}\nabla^2 + \frac{h_i A_i}{V_s}(T - T_t)\\ &= (1-\varepsilon_{eff})\rho_s \frac{\partial X}{\partial t}|\Delta H|\end{aligned} \tag{5}$$

where *ΔH* is the reaction enthalpy. Further details about the governing equations, the 2D simulation, and validation of the developed model have been presented in [8]. The reduced model, comprising the zeolite 13X–packed bed, the HTF tube, and integrated fins, along with its boundary conditions and numerical setup, is shown in Figure 2.

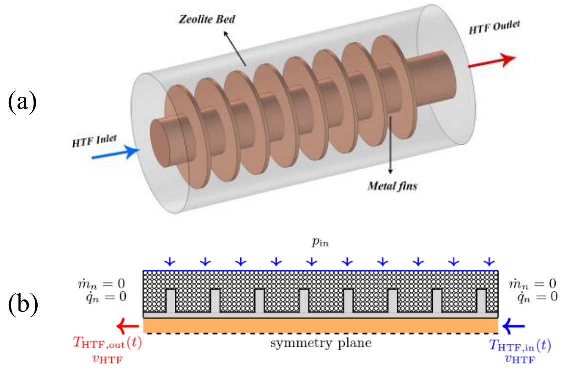

Figure 2. (a) Computational domain, (b) Boundary conditions.

Use of COMSOL Multiphysics®

The computational analysis was conducted using COMSOL Multiphysics 6.3 to solve the coupled mass and heat transfer equations. User-defined functions were developed to implement the sorption reaction kinetics and the temperature- and moisture-dependent thermophysical property correlations. The vapor flow through the porous domain was modelled using Darcy's Law interface. Coupled heat and mass transfer in the sorbent bed were resolved using the Heat Transfer in Porous Media and Transport of Diluted Species in Porous Media interfaces. The HTF flow field was computed separately using the Laminar Flow interface. To ensure high numerical accuracy, the computational domain is discretized into three distinct regions with a fine mesh composed of extremely small elements. The discretization of all governing equations follows a second-order quadratic approach. The integration between the CFD-based sorption unit model and the building energy system model was implemented using COMSOL LiveLink™ for Simulink.

Building Model Based on Simulink

The building co-simulation was implemented in MATLAB/Simulink. Standard building functions were represented with elements from the CARNOT Toolbox, including weather, house, solar collector, and thermal subsystems. The Simple House SFH15 block was adopted, by which a passive-house demand of 15 kWh/(m²·yr) is characterized [9]. The solar-collector model was developed and validated against experimental data from [10]. The STES was incorporated as a COMSOL-derived Functional Mock-up Unit (FMU).

The weather file for Athens was used [11]. In the CARNOT Simple House block, the initial indoor temperature was set to 15 °C for winter and to the ambient start temperature for other seasons. The heating system layout is illustrated in Figure 3: heat from the solar collector and the STES is delivered to the storage tank, while the space-heating loop operates with a 55–65 °C supply to radiators. An indoor set-point of 21 °C was enforced; radiator operation was triggered whenever the set-point was unmet.

The storage/domestic hot water (DHW) subsystem was implemented with Storage Type 4 and the EU hot-water tapping cycle from the CARNOT Toolbox [9]. The STES was imported as a COMSOL-derived FMU. Ancillary blocks from the CARNOT Toolbox were used for control, measurement, and hydraulics—Resident_task44, Measure_T_surface, Controller, Pump_const, and Pipe—together with supply-side auxiliaries (electric heater).

Control Strategy

Control was predominantly on–off [5]. Using the following steps: (a) selection of the active heat source for the house, (b) engagement of the backup heater if necessary, and (c) switching of the sorption reactor between adsorption and desorption. The radiator circuit was disabled when room temperature exceeded the set-point and re-enabled; if solar output was insufficient, the STES was activated; when the combined solar + STES output remained inadequate to meet the room set-point, the auxiliary heater was engaged by the backup-heater controller. Once it fell below the set-point. In the supply-priority sequence, the solar system was assigned first. The STES reactor is operated in on–off mode to regulate the building heat load. The controlled variable is the solar-collector outlet temperature T_c. During the heating period, adsorption is enabled to provide supplemental space heating alongside the solar collector (and, if required, the backup heater). During the non-heating period, desorption is initiated when $T_c > 120$°C and is disabled once T_c falls below 120°C; in the latter case, the available warm water is routed to the storage tank. The logic is summarized in Table 2. Tc denotes the solar-collector outlet temperature (°C), Q_{solar} the thermal power supplied by the solar collector (W), Q_{Demand} the building heat-demand rate (W), and $Q_{Adsorption}$ the thermal power released by the reactor during adsorption (W).

Table 2. Operating Conditions

Operating Conditions		Operation
Heating is needed	$Q_{Solar} > Q_{Demand}$	Adsorption - off Desorption - off
	$Q_{Solar} < Q_{Demand}$	Adsorption - on Desorption - off
	$Q_{adsorption} + Q_{Solar} < Q_{Demand}$	Electric heater - on
Heating is not needed	$T_c > 120$	Adsorption - off Desorption - on
	$T_c < 120$	Adsorption - off Desorption - off

Simulation Results and Discussion

The overall system in Simulink is as given in Figure 3. A variable-step, explicit Runge–Kutta (ODE45) solver was used to obtain efficient simulations while maintaining accuracy. In this paper, only the most relevant seasonal results are reported.

Winter

A cold winter day in Athens was simulated with ambient temperatures ranging from approximately 2 to 8 °C. Under these conditions, the desorption process remains inactive, while adsorption occurs because the collector produces temperatures below 120 °C, illustrated in Figure 5. In this hybrid system, the collector and sorption storage reactor jointly contribute to maintaining indoor comfort, with the room temperature stabilized at around 20°C as shown in Figure 4. The domestic hot water temperature is also kept within a comfortable range of ~40–60°C. The simulation required approximately 1,273 seconds for a single day and about 2,927 seconds for a four-day winter period.

Spring

Figure 6 illustrates the simulation results for a spring day with ambient temperatures between ~10 and ~20°C, during which the sorption storage switches between adsorption and desorption. The collector temperature rises above 120 °C, leading the storage reactor to operate in desorption. However, a delay in desorption is observed because, at times when the collector temperature exceeds 120 °C, the available solar energy is still insufficient to meet the heating demand, which activates the auxiliary electric heater. With the combined contribution of sorption reactor and solar collector, the indoor temperature is maintained at a comfortable range of 20–21°C.

Summer

The hottest summer day in Athens was selected with ambient temperatures ranging from ~26 to ~37°C. As shown in Figure 7, for most of the day, the solar collector alone meets the house's energy demand. However, during the night, when the collector temperature falls below 120°C and solar energy is insufficient, the sorption storage reactor operates in adsorption mode, contributing heat. During the daytime, when the collector temperature exceeds 120 °C and the solar energy input is greater than the house's demand, the reactor switches to desorption.

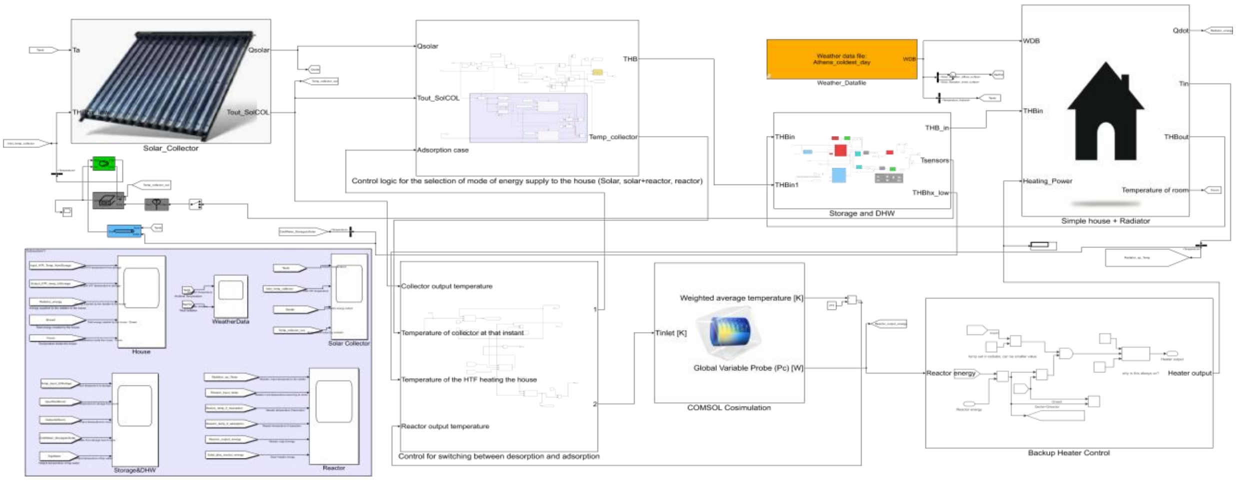

Figure 3. COMSOL–Simulink integration of a zeolite–water sorption reactor within a building energy system.

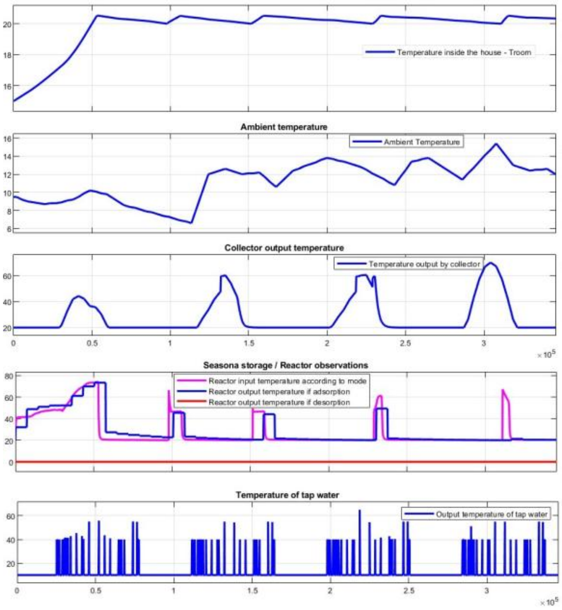

Figure 4. Simulation results for 4 days of winter.

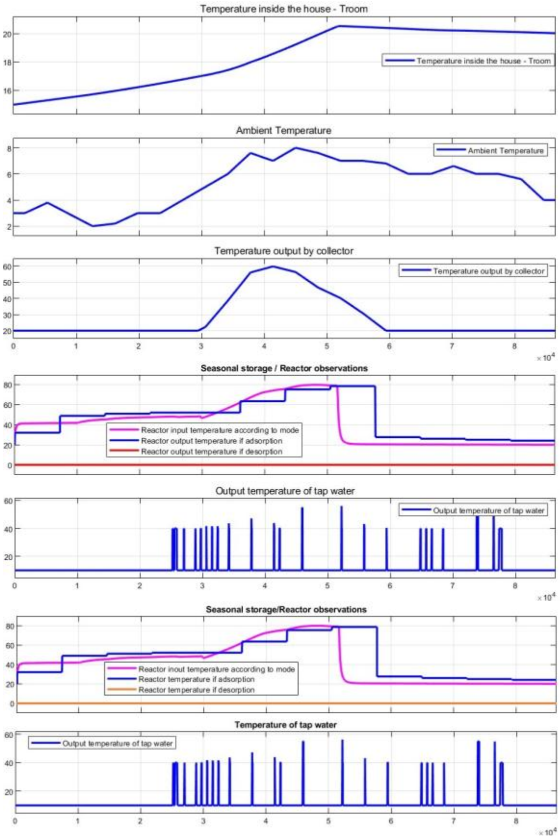

Figure 5. Simulation results for the coldest day of winter.

Autumn

Finally, Figure 8 represents the simulation results for a typical autumn day, with ambient temperatures ranging between ~16 and ~22°C. In this case, the solar collector does not reach temperatures above 120 °C, meaning the sorption storage reactor remains in adsorption mode, assisting in maintaining the room temperature at a comfortable level. he domestic hot water (DHW) supply is successfully heated to the desired range of ~40–50 °C.

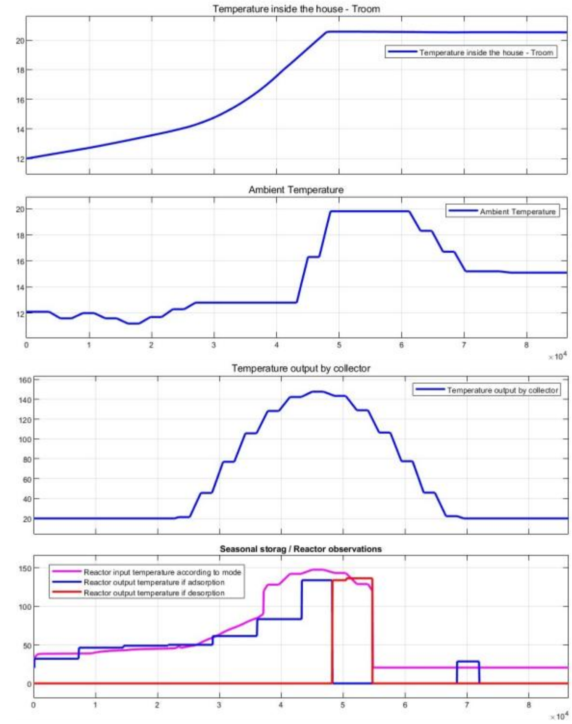

Figure 6. Simulation results for 1 day of Spring.

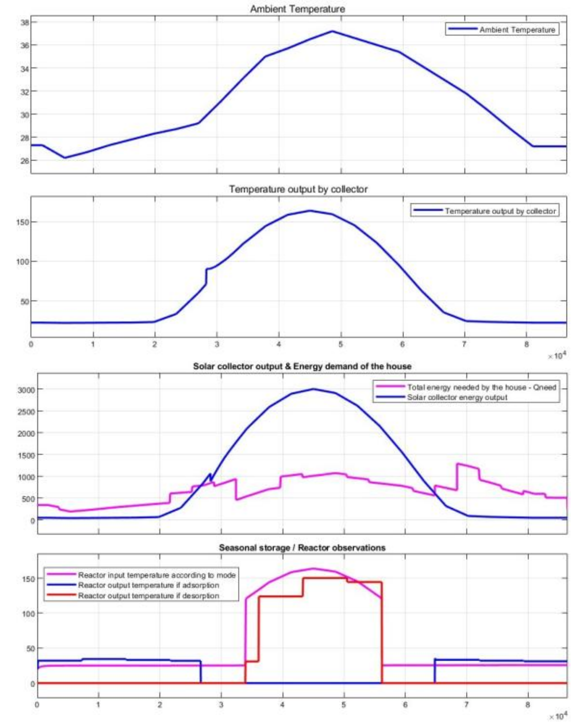

Figure 7. Simulation results for the hottest day in Summer.

Conclusions

A co-simulation framework coupling a COMSOL-derived sorption thermal energy storage (STES) reactor with a MATLAB/Simulink building model was developed and exercised under Athens weather data. An on–off supervisory strategy prioritized solar heat, then the STES, and finally backup supply, with adsorption/desorption switching based on the collector outlet temperature threshold Tc=120°C.

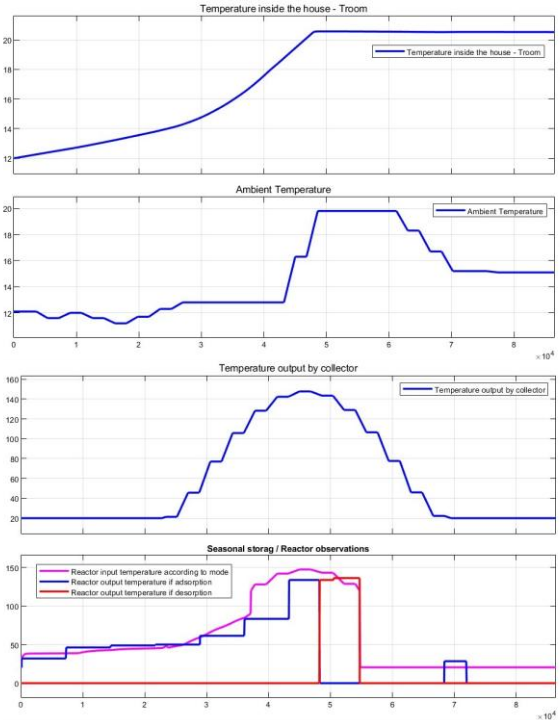

Figure 8. Simulation results for 1 day of Autumn.

Across seasons, the hybrid model reproduced expected system behavior while maintaining feasible runtimes with a variable-step ODE45 solver. In winter, the STES operated in adsorption and, together with the collector, held space temperature near 20°C and DHW in the 40–60°C range despite low solar gains. In summer, daytime desorption was triggered when Tc>120°C, demonstrating effective storage and recovery; nighttime adsorption contributed to DHW readiness when solar input fell. Spring and autumn transitions were captured with the expected alternation between adsorption and desorption, yielding stable indoor temperatures (≈20–21°C). These results indicate that (i) the selected integration architecture is technically viable, (ii) the switching logic is sufficient to maintain thermal comfort, and (iii) the co-simulation is computationally efficient.

Implications and outlook:

The presented framework provides a flexible basis for component substitution and control prototyping. Future work will focus on (1) systematic evaluation of heat-pump assistance (2) advanced control (3) design optimization of reactor/collector/storage sizing and hydraulics; (4) experimental hardware-in-the-loop validation; and (5) uncertainty and sensitivity analyses to quantify robustness under varying climates and occupant profiles.

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