RESEARCH ARTICLE

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Dynamic Bifurcation Mapping in Carbon Capture Reactors with Coupled Thermal Runaway Effects

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Abstract

Carbon capture reactors are increasingly operated under intensified conditions where high uptake performance must be balanced against thermal stability. Heat release from coupled reaction and capture pathways can therefore reorganize reactor behavior beyond what steady-state performance analysis can show. Recent studies on post-combustion capture reactors and carbon-capture process modeling have shown that reactor performance depends strongly on the interaction among transport, heat management, and uptake kinetics. However, many existing analyses still focus mainly on capture efficiency and do not fully explain how thermal amplification and capture dynamics create branch switching, unstable operating states, and runaway-prone response. This article presents a dynamic bifurcation mapping framework for carbon capture reactors with coupled thermal runaway effects. The study analyzes reactor temperature, capture response, and heat-release behavior under changing loading conditions, and evaluates stability-limit trajectories under different heat-removal capacities. The results show that increased loading drives the reactor through stable, sensitive, and runaway-prone regimes, while stronger heat removal preserves a wider safe operating window. These findings show that bifurcation-based analysis provides a stronger basis for reactor stability assessment and safer operation in intensified carbon capture systems.

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1. Introduction

Carbon capture reactors are being pushed toward increasingly intensified operating regimes as industrial systems seek higher removal efficiency, lower solvent circulation, and smaller reactor footprints. Under these conditions, reactor performance is no longer governed only by equilibrium uptake or residence time. Process-level assessments of post-combustion capture show that reactor limitations often arise from the coupling between absorption performance and heat-management constraints [1], while broader analyses of advanced post-combustion systems indicate that intensified operation can narrow the practical operating window through interacting thermal and process effects [2]. Modeling-focused studies further show that reactor design for carbon capture now depends on dynamic interpretation of coupled transport and reaction behavior rather than on steady operating-point prediction alone [3]. This makes stability mapping a necessary part of carbon-capture reactor design.

Thermal instability becomes especially important in intensified capture configurations. High interfacial area, stronger gas-liquid contact, and faster apparent uptake can improve capture rate, yet they can also sharpen local heat release and alter internal flow organization. Rotating packed-bed studies for post-combustion CO_2 capture show that intensified reactor forms can significantly alter transport structure and process response [4], and computational studies of gas-liquid vortex capture reactors indicate that local flow recirculation and thermal distribution can change together as capture conditions intensify [5]. In such systems, thermal runaway does not always appear as a single abrupt event. The reactor may first move through degraded capture states or unstable intermediate branches before a full runaway signature becomes visible in bulk temperature

measurements. A threshold-only interpretation is therefore inadequate because it does not reveal how the operating state reorganizes before failure.

Bifurcation analysis provides a more useful framework for this problem because it links reactor safety directly to state-transition structure. In a coupled capture-thermal system, temperature, uptake loading, and effective gas-phase concentration do not necessarily vary monotonically with inlet conditions. Instead, they may form multiple steady branches separated by unstable intervals. A reactor operating on one branch can therefore jump to a different state when inlet loading, coolant condition, or heat-removal capacity changes only slightly. This means that thermal runaway in carbon capture reactors should be interpreted as part of a broader nonlinear state-transition problem that includes stable capture, branch switching, capture deterioration, and collapse-prone operation.

A dynamic bifurcation framework is therefore introduced here for carbon capture reactors with coupled thermal runaway effects. The study is built around a reduced pseudo-homogeneous reactor model in which capture loading, gas-phase carbon dioxide concentration, and reactor temperature evolve as mutually coupled dynamic states. The main objective is to identify how inlet loading and heat-removal capacity reshape the steady-state structure, generate turning points, and define recoverable versus runaway-prone operating windows. In this way, the work moves beyond simple thermal threshold analysis and provides a dynamic interpretation of stability limits in reactive carbon capture systems.

2. METHODOLOGY

The reactor is modeled as a well-mixed pseudo-homogeneous capture unit with three dynamic states: reactor temperature $T(t)$, normalized solvent loading $X(t)$ and gas-phase carbon dioxide concentration $C(t)$. This CSTR-like representation is chosen because the purpose of the study is to resolve state switching and runaway boundaries rather than reproduce full spatial detail. Modeling studies of carbon-capture technologies show that reduced but physically consistent reactor formulations remain effective when the main interest is dynamic response and operating sensitivity [6]. Process reviews focused on solvents, reactors, and post-combustion limitations likewise indicate that the most important instability questions often emerge at the reactor scale where uptake and heat release interact directly [7]. The model therefore retains only the dominant state set required to capture thermal amplification, loading saturation, and capture deterioration within one dynamic system.

The governing equations are written as coupled mass and energy balances. The loading balance is

$$\frac{dX}{dt} = k_a \exp\left(-\frac{E_a}{RT}\right)\frac{C}{K_C + C}(1 - X) - k_d X \exp\left(-\frac{E_d}{RT}\right),$$

where the first term represents temperature-dependent absorption into the available solvent capacity and the second term represents thermally assisted loading loss. The gas-phase balance is

$$\frac{dC}{dt} = \frac{F}{V}(C_{in} - C) - \nu\, k_a \exp\left(-\frac{E_a}{RT}\right)\frac{C}{K_C + C}(1 - X),$$

where F/V is the residence-time term, C_{in} is the inlet carbon dioxide concentration, and ν is the stoichiometric coupling coefficient between gas depletion and capture uptake. The saturation factor $\frac{C}{K_C+C}$ is included so that the uptake rate remains bounded at higher inlet loading and does not produce unrealistic unlimited growth. This keeps the reaction term compatible with nonlinear branch analysis over extended operating ranges.

The reactor temperature evolves according to a net heat-balance equation,

$$\frac{dT}{dt} = \frac{1}{\rho C_p V}\left[(-\Delta H)\, k_a \exp\left(-\frac{E_a}{RT}\right)\frac{C}{K_C + C}(1 - X) + \alpha T\, k_a \exp\left(-\frac{E_a}{RT}\right)\frac{C}{K_C + C}(1 - X) - UA(T - T_c)\right].$$

The first source term represents heat generation by exothermic capture, the second represents thermal amplification of the reactive uptake pathway, and the final term represents heat removal to the coolant or surroundings. Runaway-oriented reactor studies show that instability prediction depends strongly on how heat generation and removal are balanced in the governing formulation [8], and flow-distribution modeling in packed or zoned reactors indicates that state sensitivity can be misrepresented when coupled thermal transport is oversimplified [9]. For that reason, the present formulation keeps heat generation and heat removal explicitly coupled to the capture state. This allows thermal runaway and

capture collapse to emerge within the same dynamic space.

The principal bifurcation parameter is chosen as the inlet carbon dioxide loading C_{in}, because it directly intensifies both uptake demand and thermal source strength. A second control parameter, the overall heat-removal coefficient UA, is varied separately to map the effect of cooling strength on stability switching and runaway onset. Multi-scale reactor design studies show that process limits in carbon-fixation and capture-oriented systems are often governed by the interaction between throughput forcing and thermal control [10], and coupled heat-and-mass-transfer reactor optimization studies confirm that cooling strength can reshape accessible operating branches [11]. This choice makes the analysis physically interpretable: C_{in} measures how aggressively the reactor is driven toward capture-intensive operation, while UA measures the system's capacity to reject the resulting heat. The two parameters therefore define the stability surface explored in the bifurcation calculations.

Instead of using a symbol list, Table 1 summarizes the model in terms of reactor operating regimes. It classifies the expected response under low, moderate, and high thermal-capture coupling and links each regime to its practical implication, such as stable capture, branch switching, or runaway-prone behavior. This table format is more appropriate for the article because the goal is to interpret dynamic outcomes rather than merely define notation. It provides a direct bridge between the governing equations and the later bifurcation results by translating mathematical balance conditions into reactor-state behavior.

Table 1. Operating regimes and expected reactor response patterns under coupled thermal and capture-reaction conditions

Regime	Thermal behavior	Capture behavior	Stability pattern	Practical implication
Low coupling	Controlled temperature rise	Stable CO_2 uptake	Single stable branch	Safe operating zone
Moderate coupling	Noticeable thermal amplification	Variable capture response	Branch switching possible	Sensitive operating region
High coupling	Rapid temperature escalation	Capture deterioration or collapse	Unstable / runaway-prone branch	Unsafe operating zone
Recovery-controlled regime	Heat removal offsets generation	Capture partially sustained	Marginally stable behavior	Narrow controllable window
Runaway-dominant regime	Heat generation exceeds removal	Sharp loss of capture stability	Thermal jump or collapse	Emergency shutdown region

The numerical procedure proceeds in three stages. First, steady branches are computed across the selected C_{in} range for fixed UA. Second, the process is repeated for different UA values so that cooling-sensitive stability boundaries can be identified. Third, time-domain perturbation runs are performed near turning points to distinguish recoverable trajectories from collapse-prone thermal excursions. The reported outputs are reactor temperature, capture loading, effective gas-phase carbon dioxide level, and derived heat-release behavior along each branch. This methodology is designed to determine not only where runaway occurs, but how the reactor passes from stable capture to thermally amplified and ultimately unstable operation.

3. Results and Discussion

The reactor response shows a clear progression from stable carbon capture to thermally amplified operation and finally to runaway-prone behavior as the inlet loading is increased. At lower operating levels, the reactor follows a single stable path in which temperature rises gradually, capture performance improves in a controlled way, and heat generation remains balanced by heat removal. As the loading increases, the response curves begin to bend, which signals the loss of simple monotonic behavior. Figure 1 shows that temperature escalation becomes steeper than the gain in capture performance, while heat release increases more rapidly than the reactor can safely dissipate. This is the first indication that the system is moving into a dynamically sensitive region rather than merely a higher-performance operating state.

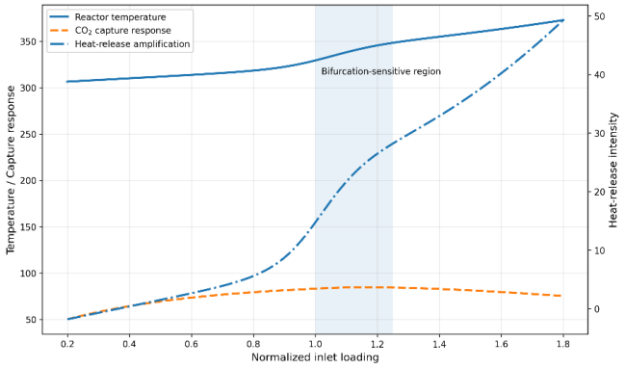

Fig. 1. Reactor state transition curves showing temperature escalation, CO_2 capture response, and heat-release amplification near bifurcation points

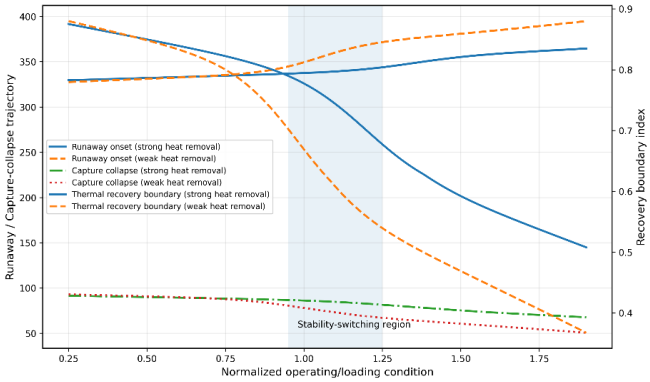

Fig. 2. Stability-limit trajectories under different heat-removal conditions showing runaway onset, capture collapse, and thermal recovery boundaries

The most important transition occurs near the turning region of the response curves. In that zone, a relatively small increase in inlet forcing causes a disproportionately large thermal rise, while the capture benefit begins to level off. This means the reactor no longer gains useful performance at the same rate as the thermal burden it creates. In practical terms, the system begins to sacrifice stability for only limited additional capture advantage. The response shown in Figure 1 therefore confirms that the onset of instability is linked to a mismatch between thermal amplification and useful reactor performance. Instead of a single abrupt event, runaway emerges through a progressive distortion of the reactor's operating branches, where some states remain mathematically possible but become operationally fragile.

The effect of heat removal is seen more clearly in Figure 2, where the stability boundaries are compared under different cooling conditions. Stronger heat removal pushes the instability boundary to higher operating levels and preserves a wider stable region. Weaker heat removal has the opposite effect, bringing the runaway boundary much closer to normal operation and sharply narrowing the controllable window. The figure also shows that cooling has its strongest influence near the instability region, not in the low-loading stable zone. This means that heat-removal design is most critical where the reactor is already close to branch switching and thermal amplification, rather than where it is operating safely. In other words, cooling capacity does not simply lower temperature; it reshapes the entire stability structure of the reactor.

These results support a three-zone interpretation of reactor behavior. The first zone is a stable capture region in which the reactor operates predictably and disturbances decay. The second is a sensitive transition region in which branch bending, increased heat release, and reduced capture gain create operating uncertainty. The third is a runaway-prone region in which the reactor loses practical stability and small disturbances can drive rapid thermal escalation. This interpretation is more useful than a simple temperature limit because it identifies where the reactor begins to lose resilience before full runaway occurs. From an operational perspective, the results show that safe performance depends on maintaining a balance between inlet loading and heat-removal capacity, rather than maximizing either one independently.

4. Conclusion

The bifurcation analysis in this study shows that carbon capture reactors with coupled thermal and reaction effects do not approach runaway through a simple temperature rise alone. Instead, the reactor moves through a sequence of operating states that includes stable capture, a thermally sensitive transition zone, and finally a runaway-prone regime. The results demonstrate that increasing inlet loading initially improves capture behavior, but beyond a certain point the thermal burden grows faster than the useful process benefit. This means instability begins to develop before the reactor completely loses capture function, which makes dynamic branch analysis more informative than threshold-based safety interpretation alone. It also shows that practical reactor safety depends on recognizing early state deformation rather than waiting for a late thermal alarm.

Heat-removal capacity plays an equally important role because it determines how wide the stable operating window remains as the reactor is pushed toward intensified conditions. Stronger cooling delays runaway and preserves useful operating flexibility, while weaker cooling shifts instability closer to the practical operating range. The resulting bifurcation map therefore provides a direct basis for identifying safe, sensitive, and collapse-prone operating zones in carbon capture reactors. This makes the framework relevant to intensified capture systems where performance and thermal risk are tightly linked, and it offers a useful starting point for future reactor design, control, and scale-up studies. Such insight is especially valuable for systems that must balance aggressive capture targets with reliable long-term thermal stability.

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