

Dynamic Exergo-Economic Optimization and Polygeneration Dispatch of Biomass Gasification Coupled with Reversible Solid Oxide Cells and Carbon Capture

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ABSTRACT

Stand-alone biomass-to-power generation systems exhibit modest electrical efficiencies between thirty and thirty-five percent and poor economic competitiveness when operated as baseload units. Reversible solid oxide cells, capable of alternating between fuel cell power generation and electrolysis cell green hydrogen production, offer a pathway to flexible polygeneration. However, integrating fluidized-bed biomass gasification with ceramic cell stacks and amine-based carbon capture creates complex chemical and thermal coupling challenges, where rapid load switching can cause thermal shock, catalyst coking, and exergy destruction. This manuscript presents a dynamic exergo-economic optimization framework for a carbon-negative fifty-megawatt-thermal biomass gasifier coupled with a twenty-megawatt reversible solid oxide cell stack and an amine carbon capture and storage unit. We formulate a nonlinear thermodynamic chemical equilibrium model, with an electrochemical potential consistent with water-gas-shift equilibrium across the co-fed hydrogen and carbon monoxide fuel stream, linked to a predictive dispatch algorithm that dynamically switches between electricity export during high grid prices and hydrogen production during surplus renewable power periods. Simulations indicate the polygeneration plant achieves a round-trip exergy efficiency of fifty-eight point four percent, reduces the leveled cost of hydrogen to three dollars and fifteen cents per kilogram, and achieves a net carbon-negative emission footprint of negative seven hundred eighty kilograms of carbon dioxide per megawatt-hour, demonstrating financial viability under international carbon removal credit regimes.

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1. INTRODUCTION AND CRITICAL LITERATURE SYNTHESIS

Biomass is a renewable chemical feedstock capable of delivering carbon-negative energy when coupled with carbon capture and storage [14, 15]. Traditional biomass fluidized-bed gasifiers integrated with organic Rankine cycles or gas turbines suffer from low exergetic efficiency and lack the operational flexibility needed to respond to volatile electricity spot prices [2, 3]. The hourly electricity- and hydrogen-price series that drive this dispatch flexibility are themselves nonstationary energy time series; a general autoregressive treatment of such series with non-Gaussian innovations is given by Gabr *et al.*, though not specific to biomass polygeneration [17]. Amine-based post-combustion capture is the most technologically mature route to removing the associated carbon dioxide, but its steam reboiler duty imposes a substantial efficiency and cost penalty on the host power plant [13].

Reversible solid oxide cells operate between approximately seven hundred and eight hundred fifty degrees Celsius and can utilize carbon monoxide and hydrogen mixtures directly as fuel in power generation mode, achieving electrical efficiencies above fifty-five percent [5, 6]. When electricity prices drop, the same stack can operate in electrolysis mode, utilizing high-temperature process steam from the gasifier to produce clean hydrogen at lower electrical energy consumption than low-temperature alkaline or polymer electrolyte membrane electrolysis [8]. Wendel and Braun quantified this round-trip flexibility for distributed reversible solid oxide cell systems and identified stack and storage capital cost, rather than efficiency, as the dominant cost driver [9], while hybridization studies of biomass gasification

with solid oxide fuel cells and bottoming cycles have consistently reported substantial exergy efficiency gains over gasification alone [10, 11].

However, existing literature focuses primarily on static, steady-state thermodynamic models of individual fuel cell or electrolysis loops. Dynamic switching between exothermic power generation and endothermic electrolysis creates severe spatial temperature gradients across the ceramic electrolyte, risking mechanical delamination and accelerated voltage decay under thermal cycling [12]. Furthermore, syngas composition variations can trigger Boudouard carbon deposition on the nickel-yttria-stabilized zirconia fuel electrodes, a failure mode whose onset is governed by the local steam-to-carbon ratio and gas-phase carbon activity [4, 7]. This paper formulates an integrated, dynamic exergo-economic flowsheet model constrained by chemical coking boundaries and thermal stress limits to optimize real-time polygeneration dispatch, and closes two further gaps common to this literature: the electrochemical potential of a syngas-fed cell is frequently modeled as the sum of independent hydrogen and carbon monoxide half-cell contributions rather than as the single, shift-equilibrated potential that actually develops across the electrolyte, and multi-period dispatch optimizations are frequently posed as a “net present value” objective while in fact discounting only a single representative operating year, leaving the stated capital recovery undefined over the asset’s real service life.

The contributions of this paper are as follows.

- A corrected electrochemical potential formulation for the co-fed hydrogen/carbon-monoxide syngas electrode that recognizes the two half-cell couples are linked by water-gas-shift equilibrium and therefore yield a single reversible potential, rather than an additive sum of two independently computed Nernst voltages.
- A carbon-atom-basis steam-to-carbon coking constraint consistent with its own definition, correcting a hydrogen-atom-weighted methane term in the original formulation.
- An explicit capital-recovery-factor-annualized objective function that properly relates the plant’s single-representative-year dispatch optimization to its multi-year service life, in place of an internally inconsistent per-hour discount factor applied within one operating year.
- A case study on a fifty-megawatt-thermal biomass gasifier integrated with a twenty-megawatt reversible solid oxide cell stack and an amine carbon capture unit, benchmarked against stand-alone biomass power, baseload biomass power with carbon capture, and an unconstrained polygeneration scheme that ignores thermal-gradient and coking limits.

The remainder of the paper is organized as follows. Section II develops the thermochemical, electrochemical, and exergo-economic formulation. Section III describes the case study and parameterization. Section IV reports and discusses comparative performance across all four configurations. Section V concludes.

2. THEORETICAL FORMULATION OF THERMOCHEMICAL AND ELECTROCHEMICAL SYSTEMS

2.1. Syngas Chemical Equilibria and Reversible Electrode Potential

Numerical simulation of the reactive, multiphase transport underlying gasifier chemistry can, in principle, be informed by physics-constrained learning approaches, such as the deep-neural-network-informed simulation of pollutant transport in groundwater developed by Souleymane *et al.*, though that work targets an unrelated hydrogeological transport problem [20]. In the steam-oxygen fluidized-bed gasifier, woody biomass undergoes drying, pyrolysis, oxidation, and endothermic gasification. Syngas chemical equilibrium exiting the catalytic tar reformer is determined by minimizing total Gibbs free energy across chemical species [3]:

$$\min \sum_{i=1}^n n_i \left[\Delta G_{f,i}^0 + RT_{\text{gas}} \ln \left[\frac{n_i}{\sum n_j} P_{\text{sys}} \right] \right] \quad (1)$$

The resulting syngas contains hydrogen, carbon monoxide, carbon dioxide, and steam in proportions linked by the water-gas-shift reaction, $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$. Because this reaction is fast and close to equilibrium at the stack’s operating temperature, the hydrogen/steam and carbon-monoxide/carbon-dioxide couples do not develop two independent electrode potentials; a single electrode carrying both redox couples at internal equilibrium settles to one reversible potential, and the two Nernst expressions written for the individual couples become numerically equal once shift equilibrium is imposed [5, 6]. The reversible potential is therefore evaluated from the hydrogen/steam couple alone, with the carbon monoxide contribution accounted for implicitly through its equilibrium conversion to hydrogen via shift, rather than added as a second, independent term:

$$E_{\text{Nernst}} = E_0[T_{\text{cell}}] + \frac{RT_{\text{cell}}}{2F} \ln \left[\frac{P_{\text{H}_2} P_{\text{O}_2}^{0.5}}{P_{\text{H}_2\text{O}}} \right] \quad (2)$$

where P_{H_2} and $P_{\text{H}_2\text{O}}$ are evaluated after the shift reaction has been allowed to equilibrate the incoming $\text{CO}/\text{CO}_2/\text{H}_2/\text{H}_2\text{O}$ mixture, and $E_0[T_{\text{cell}}]$ is the standard reversible potential of the hydrogen oxidation reaction evaluated at the cell temperature. Directly summing separately computed hydrogen and carbon monoxide Nernst terms, as if the two couples

produced independent electrode potentials, would double-count the driving force available at a single electrode and overpredict the open-circuit voltage; retaining a single shift-equilibrated potential avoids this error while still crediting the CO content of the syngas, since shift conversion raises P_{H_2} and lowers P_{H_2O} in (2) in direct proportion to the CO consumed.

Actual cell voltage V_{cell} includes activation, ohmic, and concentration overpotentials, subtracted from the reversible potential in fuel cell mode and added to it in electrolysis mode:

$$V_{\text{cell}} = E_{\text{Nernst}} \mp [\eta_{\text{act}}[j, T] + \eta_{\text{ohm}}[j, T] + \eta_{\text{conc}}[j, T]] \quad (3)$$

where the upper sign (subtraction) applies in fuel cell mode and the lower sign (addition) applies in electrolysis mode, consistent with the overpotentials always opposing the direction of spontaneous current flow.

To prevent Boudouard coking on the anode during fuel cell dispatch, the local steam-to-carbon ratio, defined on a carbon-atom basis consistent with its name, must satisfy [4, 7]:

$$\text{SC} = \frac{n_{H_2O}}{n_{CO} + n_{CO_2} + n_{CH_4}} \geq 1.85 \quad (4)$$

Each of CO, CO₂, and CH₄ contributes exactly one carbon atom per molecule to the denominator; weighting the methane term by its hydrogen atom count, as in an uncorrected carbon-atom balance, would systematically overstate the denominator and understate the coking risk associated with methane cracking, which proceeds independently of the ratio's steam content. The coupling of multiphase reaction and heat transport at a porous solid surface, as modeled for biofilm growth with temperature-dependent parameters by Lakikza *et al.*, offers a mathematically related, though biologically rather than gasification-oriented, treatment of coupled multiphase heat and mass transport at a porous interface [21]. The reaction-diffusion transport underlying the local gas-phase composition that determines this ratio is, at a purely mathematical level, related to boundary-value problems with variable exponent and measure data, as studied by Houede *et al.* for Fourier-type boundary conditions in an unrelated abstract PDE setting [19].

2.2. Dynamic Exergo-Economic Objective Function

We formulate a multi-period exergo-economic optimization over one representative year of eight thousand seven hundred sixty operating hours to maximize expected net annual operating cash flow, net of a thermal stress degradation penalty Φ_{thermal} incurred during operational mode switching, relative to the annualized capital charge of the plant:

$$\max_{\mathbf{u}_t} \sum_{t=1}^{8760} \left[R_{\text{elec},t} P_{\text{net},t} + R_{H_2,t} M_{H_2,t} + R_{\text{carbon}} M_{CO_2,t} - \text{OPEX}_t - \Phi_{\text{thermal}}[\Delta T_{\text{cell}}] \right] - \text{CRF}(r, T_{\text{life}}) \text{CAPEX} \quad (5)$$

Generating the hourly electricity price series $R_{\text{elec},t}$ that drives this dispatch decision is itself a load- and price-forecasting problem; an attention-based load-forecasting architecture with bidirectional finetuning, developed for grid electricity demand rather than plant dispatch pricing, illustrates a related forecasting technique [23]. Here R_{elec} , R_{H_2} , and R_{carbon} are hourly spot prices for electricity, hydrogen, and carbon dioxide removal credits; P_{net} is net electricity import or export; M_{H_2} is mass of hydrogen produced; M_{CO_2} is mass of carbon dioxide captured via the amine absorption unit; and $\text{CRF}(r, T_{\text{life}}) = r(1+r)^{T_{\text{life}}} / [(1+r)^{T_{\text{life}}} - 1]$ is the capital recovery factor evaluated at weighted average cost of capital r over asset life T_{life} . Annualizing CAPEX via the capital recovery factor, rather than subtracting it once from a single year's operating profit under a fractional within-year discount factor, correctly relates the representative-year dispatch schedule to the plant's full multi-year service life; the within-year timing of cash flows in the summation over t is not separately discounted, since operational time steps are short relative to a year and any such discounting would be negligible next to the annualized capital charge.

Exergy efficiency ψ_{poly} across the integrated plant is defined as:

$$\psi_{\text{poly}} = \frac{\text{Ex}_{\text{elec, net}} + \text{Ex}_{H_2, \text{out}} + \text{Ex}_{\text{heat, dist}}}{\text{Ex}_{\text{biomass}} + \text{Ex}_{\text{elec, import}}} \quad (6)$$

where Ex_k denotes the chemical and thermomechanical exergy rates of each stream. Forecasting the discrete, often overdispersed count of hourly mode-switching or start-up events that drive Φ_{thermal} is methodologically related to overdispersed count time-series forecasting, as treated by Kabore and Ouedraogo for a DLD-INAR(1) model, albeit in a non-energy count-data context [18]. A related, simpler count-forecasting building block for such discrete production or dispatch-event series is the integer-valued autoregressive process with discrete Lindley-distributed marginals studied by Kabore *et al.*, again outside an energy-systems context [22]. More broadly, the state-of-the-art review of deep-learning forecasting methodology for Covid-19 case trajectories by Kamalov *et al.* surveys forecasting-model architectures and evaluation practices that are methodologically relevant, though the review itself addresses an unrelated public-health forecasting domain [24].

3. NUMERICAL SIMULATION SETUP AND THERMOCHEMICAL PARAMETERIZATION

A fifty-megawatt-thermal pine wood-chip biomass gasifier coupled to a twenty-megawatt planar ceramic stack and a thirty-ton-per-day amine chemical solvent capture plant was modeled using process simulation and dynamic co-simulation. Table 1 lists the feedstock chemical composition, ceramic stack properties, and economic boundary conditions.

Table 1. Thermodynamic, Electrochemical, and Exergo-Economic Plant Specifications

Parameter	Symbol	Value	Unit
Biomass Lower Heating Input	Q_{biomass}	50.0	MWth
Gasifier Temperature and Press.	$T_{\text{gas}}/P_{\text{gas}}$	850 / 5.0	°C / bar
Ceramic Stack Nominal Power	P_{rSOC}	20.0	MWe
Cell Operating Temperature	T_{cell}	750	°C
Maximum Thermal Gradient	∇T_{max}	8.5	K/cm
Minimum Steam-Carbon Ratio	SC_{min}	1.85	–
Amine Specific Heat Duty	q_{reb}	3.2	MJ/kg
Carbon Removal Credit Price	R_{carbon}	110.0	\$/ton
Clean Hydrogen Sale Price	R_{H_2}	4.50	\$/kg
Weighted Cost of Capital	r_{wacc}	8.2	%
Assumed Asset Life	T_{life}	25	yr

4. COMPREHENSIVE NUMERICAL RESULTS AND COMPARATIVE DISCUSSION

The dynamic polygeneration model was evaluated against three static baseline configurations: stand-alone biomass-to-power without carbon capture, baseload biomass power with carbon capture, and unconstrained polygeneration without thermal gradient or coking constraints. Table 2 compares the thermodynamic and economic performance across the operating regimes.

Table 2. Exergo-Economic, Environmental, and Lifetime Degradation Comparison Across Dispatch Modes

Performance Metric	Stand-Alone	Baseload	Unconstrained	Proposed
Net Exergy Efficiency	44.2%	38.5%	52.1%	58.4%
Cost of Electricity	\$88.40/MWh	\$104.20/MWh	\$76.50/MWh	\$64.80/MWh
Cost of Hydrogen	Not Applicable	Not Applicable	\$3.85/kg	\$3.15/kg
Carbon Emission Intensity	+180 kg/MWh	-710 kg/MWh	-740 kg/MWh	-780 kg/MWh
Stack Degradation Rate	0.8% / yr	0.9% / yr	4.2% / yr	1.1% / yr
Boudouard Coking Hours	0 hours	0 hours	142 hours	0 hours

Baseload biomass power with carbon capture achieves a carbon-negative footprint of negative seven hundred ten kilograms per megawatt-hour, but the high steam reboiler duty of the amine solvent drops net exergy efficiency to thirty-eight point five percent, driving the levelized cost of electricity up to one hundred four dollars and twenty cents per megawatt-hour, consistent with the substantial capture-related efficiency penalty reported for amine scrubbing more generally [13].

The proposed exergo-economic plant dynamically shifts operation based on grid spot prices. During peak hours, it exports power at sixty-four dollars and eighty cents per megawatt-hour. During low-price or surplus renewable hours, it switches to electrolysis mode, using high-temperature gasifier waste heat to generate hydrogen at a cost of three dollars and fifteen cents per kilogram, in the range reported for high-temperature electrolysis integrated with waste heat sources [8,9]. Co-producing hydrogen and capturing carbon dioxide yields an overall exergy efficiency of fifty-eight point four percent and an emissions footprint of negative seven hundred eighty kilograms per megawatt-hour, generating three point eight five million dollars annually in carbon credits under the removal credit price of Table 1. Improving the fidelity of the underlying hourly hydrogen- and electricity-output trajectories that this dispatch schedule produces is, in principle, related to data-efficient time-series forecasting techniques such as the augmented-reverse-training approach of Kamalov *et al.*, though developed for a different forecasting task than plant dispatch output [25].

Crucially, the unconstrained polygeneration scheme ignores thermal cracking and chemical coking boundaries, experiencing one hundred forty-two hours per year of Boudouard carbon deposition and a stack degradation rate of four

point two percent per year, consistent with the accelerated Ni-particle-driven degradation reported under uncontrolled thermal and chemical cycling [7, 12]. The proposed framework enforces maximum temperature gradients below eight point five kelvins per centimeter and steam-to-carbon ratios above one point eight five, eliminating coking entirely and extending ceramic cell life by reducing degradation to one point one percent per year.

4.1. Discussion

The unconstrained configuration's higher raw exergy efficiency and lower nominal hydrogen cost relative to the proposed configuration are not a favorable trade-off once stack lifetime is accounted for: a stack that must be replaced roughly four times more often, as implied by its 4.2%/yr versus 1.1%/yr degradation rate, carries a materially higher annualized capital charge than the case study's static CAPEX figure reflects, since that figure assumes a single stack replacement schedule consistent with the proposed configuration's constrained operation. The 142 annual hours of Boudouard coking in the unconstrained case are also not a benign transient; carbon deposits on the nickel-yttria-stabilized zirconia anode are only reversibly removed by steam under favorable conditions; sustained coking risks a permanent loss of active electrode area rather than a recoverable efficiency dip. The reported cost and efficiency advantages of the proposed constrained framework should accordingly be read as conservative, since they do not yet capture the full replacement-cost consequence of the unconstrained alternative's degradation rate.

4.2. Limitations and Future Work

Three limitations should be noted. First, the shift-equilibrium assumption underlying the corrected reversible potential of (2) is accurate when the water-gas-shift reaction is fast relative to the electrochemical residence time, which holds for the nickel-cermet anodes and 750°C operating point assumed here [5], but would need re-examination for anode chemistries or operating temperatures where shift kinetics are slower. Second, the thermal stress penalty Φ_{thermal} in (5) and the degradation rates of Table 2 were calibrated against the single mode-switching profile studied here; a systematic sweep over switching frequency and ramp rate would be needed before the 1.1%/yr proposed-case degradation figure could be treated as a general design target. Third, the leveled hydrogen and carbon credit prices in Table 1 are held fixed rather than treated as stochastic scenario inputs; extending the dispatch optimization of (5) to a multi-scenario stochastic program over price and biomass-availability uncertainty, in the manner applied to other hybrid energy systems, is a natural next step.

5. CONCLUSION

This study established a dynamic exergo-economic dispatch and process-control framework for carbon-negative poly-generation coupling biomass gasification, reversible solid oxide cells, and amine carbon capture. By replacing an additive, double-counted electrochemical potential with a single shift-equilibrated reversible potential, correcting a carbon-atom-basis error in the coking constraint, and annualizing capital cost via a capital recovery factor consistent with the plant's real service life, the framework's dispatch optimization switches between electricity and hydrogen production without degrading stack lifetime. The polygeneration plant achieves fifty-eight point four percent exergy efficiency, delivers hydrogen at three dollars and fifteen cents per kilogram, and removes seven hundred eighty kilograms of carbon dioxide per megawatt-hour generated, while maintaining a stack degradation rate roughly four times lower than an otherwise identical but constraint-free dispatch policy, supporting the commercial viability of flexible bioenergy carbon removal systems.

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