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Operationalizing Iso 14064-1:2018 In Energy-Intensive Process Industries: A Methodological Framework Bridging Process Simulation and Auditable Scope 1–2 GHG Inventories

JOSHUA SELEUESE OKOJIE[1], RASHEEDAH FOLA ABIOYE[2]
[1]*Bremerhaven, Germany*
[2]*New Era Geosciences, Lagos, Nigeria*

Abstract- The corporate quantification of greenhouse gas (GHG) emissions has matured into a critical interface between climate policy, financial disclosure, and engineering practice, particularly within sectors where thermal energy demand and material transformation drive disproportionate atmospheric loadings. This study develops a structured methodological architecture that integrates first-principles process simulation with the directly attributable and energy-related categories prescribed by the revised international standard for organisational GHG accounting. Drawing upon a synthesis of regulatory texts, life cycle inventory scholarship, and process systems engineering literature, the paper articulates a four-tier procedural pipeline encompassing boundary delineation and consolidation choice, calibrated steady-state simulation grounded in measured plant data, systematic translation of simulator outputs into emission factors and activity data, and uncertainty propagation aligned with verification-grade evidentiary thresholds. The framework reconciles deterministic engineering computations with the probabilistic and disclosure-oriented expectations of third-party assurance, thereby resolving a long-standing tension between bottom-up engineering accuracy and top-down reporting compliance. Comparative discussion of cement, integrated steel, hydrocarbon refining, and bulk petrochemical archetypes demonstrates the framework's transferability and surfaces sector-specific pitfalls relating to fugitive emissions, allocation of cogenerated energy, and the categorisation of grid-purchased versus self-generated electricity. The paper argues that the convergence between simulation-based mass and energy balances and standard-conformant inventories is not merely procedural but constitutes a substantive epistemic shift in how industrial decarbonisation claims become defensible. Implications are drawn for verifiers, regulators, and corporate sustainability managers, particularly in jurisdictions where reporting infrastructures remain nascent. The framework offers a replicable scaffolding for translating complex thermochemical realities into legible, auditable carbon disclosures.

Keywords: Corporate Carbon Accounting; Verification Assurance; Mass and Energy Balance Modelling; Emission Factor Derivation; Uncertainty Propagation; Industrial Decarbonization

I. INTRODUCTION

The accelerating volumes of plastic packaging entering global material flows have transformed what was once an obscure industrial waste stream into a central preoccupation of environmental policy, corporate sustainability strategy, and public-health discourse. Cumulative global production of polymers had exceeded 8.3 billion metric tonnes by the middle of the previous decade, with packaging consistently identified as the largest single application sector and the dominant contributor to short-lived plastic waste (Geyer, Jambeck & Law, 2017). The persistence of polymeric materials in terrestrial and marine environments, combined with the magnitude of these throughputs, has catalysed a paradigmatic shift from linear consumption logic toward closed-loop models, in which post-consumer plastic is no longer treated as a residual liability but as a recoverable feedstock (Ellen MacArthur Foundation, 2016). Within this re-framing, post-consumer recycled (PCR) polymers have emerged as a pivotal material category, simultaneously serving climate-mitigation objectives, brand-led sustainability commitments, and statutory recycled-content mandates that are proliferating across the European Union, the United Kingdom, and a growing constellation of national jurisdictions.

The conceptual elegance of circularity, however, belies a substantive operational tension that scholars have increasingly foregrounded. The circular economy, while promoted as an integrative paradigm, accommodates competing definitions and divergent operationalisations whose policy and material implications are often only loosely coupled, with consequences that ripple through downstream design, procurement, and compliance functions (Kirchherr, Reike & Hekkert, 2017). Nowhere is this tension more acute than in consumer-goods packaging, where the material substitutability of virgin and recycled polymers must be reconciled with stringent migration limits, food-contact compliance obligations, and the legacy chemistry that recycled feedstocks inevitably carry.

The chemical inventory of post-consumer polymer streams constitutes the first axis of this tension. Empirical surveys of legacy and contemporary plastic additives have documented several thousand functional substances, including plasticisers, brominated flame retardants, stabilisers, and non-intentionally added substances, whose migration potential persists across multiple recycling cycles (Hahladakis et al., 2018). Targeted analytical campaigns have identified phthalate esters and other regulated substances of very great concern in mechanically recycled polyolefin and polyethylene terephthalate fractions at concentrations that complicate downstream food-contact and toy-grade applications (Pivnenko et al., 2016). Reviews of recycling technologies further confirm that mechanical processing, while economically dominant, exerts limited influence on chemical purification, whereas chemical and solvent-based recycling routes capable of restoring near-virgin specifications remain commercially constrained (Ragaert, Delva & Van Geem, 2017). The cumulative implication is that PCR adoption cannot be evaluated on tonnage or carbon metrics alone; it must be tested against the chemical-safety thresholds embedded in product-specific regulatory regimes.

Among such regimes, the European Union's Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) framework provides the most consequential and transboundary benchmark. REACH inverts the historical burden of proof, obliging manufacturers and importers to characterise the hazards of substances placed on the market and to demonstrate the controlled use of those identified as substances of very great concern (Williams, Panko & Paustenbach, 2009). Its applicability to recyclates, particularly through the interaction of waste end-of-status determinations with substance-in-article notification duties, has generated persistent interpretive uncertainty for converters and brand-owners. Parallel concerns over migration into food matrices have prompted refined guidance on the circular use of food-contact materials, in which residual contaminant management is treated as the principal gating constraint rather than a peripheral compliance task (Geueke, Groh & Muncke, 2018).

The challenge is intensified, rather than attenuated, when the analytical lens shifts to lower-income and emerging-market contexts. Substance-flow studies in Nigeria have documented elevated stocks of brominated and other restricted compounds in plastic streams sourced from end-of-life electrical and electronic equipment, with uncontrolled co-mingling exposing workers and consumers to bioaccumulative hazards (Babayemi et al., 2015). The structural inadequacies of municipal waste governance, exposed during the Covid-19 disruption, further demonstrated how informal-sector dependencies can both enable and frustrate circular ambitions in West African economies (Nzeadibe & Ejike-Alieji, 2020). These dynamics intersect with longstanding distributive concerns regarding sustainability transitions and the differential exposure of African populations to externalised environmental risks (Adeojo & Osinibi, 2016).

Reconciling these intersecting pressures demands more than narrative acknowledgement; it requires a structured decision logic capable of integrating chemical-safety screening, lifecycle greenhouse-gas accounting, and forward-looking regulatory-risk evaluation within a single, defensible analytical scaffold. The present review develops the conceptual basis for such a framework, situating it within the converging trajectories of European chemicals law, science-based emissions targets, and the operational realities confronting consumer-goods manufacturers across the Global North and South.

1.1 Background of the Study

Anthropogenic interference with the climate system has become the defining environmental concern of the twenty-first century, with industrial activity occupying a central role in both diagnosing the problem and constructing plausible mitigation pathways. The carbon embedded in international trade and the asymmetric distribution of production-based versus consumption-based emissions illustrate that responsibility for atmospheric loadings cannot be apportioned through national accounts alone, and that the firm-level inventory has become an indispensable instrument of climate governance (Hertwich & Peters, 2009). The mitigation literature consolidated in successive assessment cycles emphasises that the industrial sector accounts for a sizeable fraction of direct greenhouse gas (GHG) emissions and an even larger share once electricity and heat consumption are attributed to it, with cement, iron and steel, refining, and bulk chemicals dominating the energy-intensive subset (Edenhofer et al., 2014). The conceptual scaffolding through which firms render their atmospheric impact intelligible to investors, regulators, and civil society has crystallised around the notion of the carbon footprint, which, although ostensibly intuitive, conceals significant methodological choices regarding system boundaries, data sources, and reporting conventions (Wiedmann & Minx, 2008). Benchmarking exercises across industrialised and emerging economies have demonstrated that energy intensity in heavy industry varies dramatically across firms, technologies, and geographies, suggesting that a credible inventory must be sensitive to operational realities rather than reliant on aggregate proxies (Saygin et al., 2011). The convergence of these strands has rendered the corporate inventory simultaneously a technical artefact and a political document, demanding methodological sophistication commensurate with its growing decisional weight. Recognition of this dual character has progressively reshaped expectations of corporate disclosure, with investors, regulators, and standard-setting bodies increasingly demanding that reported figures be reconcilable with underlying engineering realities rather than constituting accounting outputs detached from physical operations.

1.2 Conceptual and Regulatory Context

The institutional architecture of corporate carbon accounting has evolved through layered standardisation, beginning with the publication of the original protocol that introduced the now-canonical tripartite categorisation of direct, energy-related indirect, and value-chain emissions (WRI & WBCSD, 2004). Subsequent guidance refined the treatment of purchased electricity, recognising that the choice between location-based and market-based reporting profoundly alters the disclosed footprint and may incentivise procurement of contractual instruments rather than substantive operational change (WRI & WBCSD, 2015). Within this evolving landscape, the revised international specification for organisational quantification represents a consequential reformulation, replacing the earlier scope nomenclature with categories of direct, indirect from imported energy, and indirect from transportation, products used, products from the organisation, and other sources, while strengthening the requirements for documented evidence and uncertainty disclosure (ISO, 2018). A systematic synthesis of the carbon accounting literature reveals that, despite the proliferation of standards, foundational concerns about consistency, comparability, and verifiability remain partially unresolved, and that practitioners frequently confront tensions between the prescriptive logic of accounting and the indeterminate physics of industrial processes (Stechemesser & Guenther, 2012). These tensions are particularly acute in process industries where the boundaries between scopes are blurred by waste heat recovery, on-site cogeneration, by-product fuels, and integrated chemical complexes, all of which complicate the otherwise clean separation between direct combustion and purchased energy. Resolving these complications demands an interpretive apparatus that is both standard-conformant and engineering-literate. The asymmetry between the prescriptive certainty implicit in inventory disclosure and the operational variability inherent in continuous-process operations introduces a methodological strain that successive standardisation efforts have only partially addressed, and the present revision raises rather than answers many of the most consequential questions about how engineering evidence should be marshalled to satisfy reporting requirements. Practitioners are accordingly compelled to construct interpretive bridges between regulatory categories and physical reality, and the durability of those bridges depends critically on the rigour with which underlying engineering computations are documented and exposed to independent scrutiny.

1.3 Process Simulation as Auditable Evidence

Process simulation has long served as the cognitive backbone of chemical engineering practice, providing an integrated environment in which thermodynamic relations, reaction kinetics, and unit-operation models converge to predict steady-state and dynamic behaviour of complex installations (Smith, 2005). Modern integrated design platforms allow engineers to specify feed compositions, operating pressures, temperatures, and equipment configurations, then solve simultaneously for the streams, duties, and material conversions that characterise the plant's thermochemical reality, producing detailed mass and energy balances that are demonstrably consistent with conservation laws (Dimian, Bildea & Kiss, 2014). The pedagogical and practical literature on simulation tools further emphasises that, when calibrated against measured operating data, the simulator becomes a digital twin whose outputs may be interrogated, audited, and traced to first principles, thereby offering an evidentiary substrate that mere meter aggregation cannot match (Foo, 2017). The implication for greenhouse gas reporting is striking: a simulator validated against plant performance can generate emission factors and activity data that are both internally consistent and externally defensible, while simultaneously enabling counterfactual analyses that quantify the inventory consequences of process modifications. Yet the literature on corporate carbon accounting has only partially absorbed this engineering capability, frequently treating simulation as an optimisation aid rather than as an evidentiary instrument. Bridging that conceptual gap is precisely the contribution that the present analysis seeks to make. The paradigmatic shift entailed in repositioning simulation from a design-phase tool to an ongoing inventory-substantiating apparatus carries significant implications for how plants are instrumented, how operating data are archived, and how engineering teams interface with sustainability reporting functions, and it requires the development of disciplinary protocols that have, to date, been articulated only sporadically across the relevant scholarly and professional literatures.

1.4 Aim, Objectives, and Scope

This study aims to articulate, justify, and elaborate a coherent methodological framework that enables organisations operating capital-intensive thermochemical installations to translate the engineering reality of their plants into greenhouse gas inventories that conform to the revised international standard while remaining defensible under the scrutiny of independent verification. The work pursues four specific objectives. First, it consolidates the conceptual and regulatory foundations of organisational carbon accounting, attending in particular to the categorical reformulation introduced in the 2018 revision and the assurance expectations that accompany it. Second, it synthesises the process systems engineering literature on calibrated simulation, mass and energy balance closure, and emission factor derivation, identifying the operational pathways through which simulator outputs may be transformed into inventory line items. Third, it constructs an integrated procedural pipeline that sequentially addresses boundary delineation, simulation calibration, output translation, and uncertainty propagation, demonstrating how each stage produces evidence amenable to third-party scrutiny. Fourth, it considers the comparative implementation of the framework across cement, integrated steel, hydrocarbon refining, and petrochemical archetypes, surfacing sector-specific challenges. The scope is deliberately confined to direct emissions and emissions arising from imported energy, since these constitute the operationally controllable categories most amenable to engineering computation, while value-chain emissions, although consequential, are bracketed for separate treatment owing to their reliance on supplier-specific data. The geographic emphasis privileges energy-intensive process industries operating in both mature regulatory environments and emerging-market jurisdictions, recognising that the technical questions of inventory construction transcend institutional context even where the assurance ecosystems differ in maturity.

II. THEORETICAL AND REGULATORY FRAMEWORK OF ORGANISATIONAL GHG QUANTIFICATION

The theoretical foundation upon which the contemporary corporate inventory rests is, in the first instance, the architecture of national greenhouse gas accounting articulated through the methodological volumes of the Intergovernmental Panel on Climate Change, which formalised tier-based approaches differentiated by the granularity of activity data and the specificity of emission factors (IPCC, 2006). These tiers distinguish between default factors derived from broad sectoral averages, country-specific factors reflecting national fuel characteristics, and facility-specific factors derived from direct measurement or detailed engineering models, with progressively higher tiers offering reduced uncertainty at the cost of greater data demands. Although developed for national reporting under the United Nations Framework Convention on Climate Change, these tiers have been recursively absorbed into corporate guidance and exert continuing influence on how organisations conceptualise the choice between simple, calculation-based, and measurement-based approaches.

The corporate-level translation of these methodological principles found its most influential expression in sectoral protocols that addressed industry-specific complexities. The cement sector, in particular, developed a dedicated accounting and reporting standard that codified the treatment of clinker calcination, alternative fuels, and biomass combustion, thereby providing a template that subsequent sectoral initiatives have emulated (WBCSD, 2005). Cross-sectoral debates about the proper scope of corporate accounting were sharpened by the contrast between consequential and attributional analytical orientations, with the former concerned with marginal effects of decisions and the latter with the apportionment of existing emissions among reporting entities, a distinction that retains profound implications for boundary setting (Brander et al., 2008).

Beyond the technical apparatus of measurement and computation, the institutional rise of carbon accounting must be situated within the broader trajectory of environmental accounting scholarship. The discipline of accounting was challenged to confront its environmental responsibilities, with calls for a substantive reorientation that would transcend the merely cosmetic incorporation of ecological concerns into existing reporting templates (Hopwood, 2009). Empirical investigations of carbon accounting in practice have demonstrated that the production of inventory numbers involves negotiation among engineers, accountants, sustainability officers, and verifiers, with each constituency bringing distinct epistemic standards to the encounter, and the resulting numbers reflecting compromises rather than the application of a single coherent measurement logic (Bowen & Wittneben, 2011).

Studies of leading firms have shown that internal carbon management practices vary substantially in sophistication, with some organisations integrating carbon information into operational decision-making while others maintain it as a peripheral compliance artefact (Burritt, Schaltegger & Zvezdov, 2011). The historical perspective offered by case studies of environmental accounting implementation reveals that the introduction of new disclosure regimes can either catalyse genuine change or be appropriated to legitimate existing practices without substantively altering them, an insight that retains its salience as standards proliferate (Larrinaga-González & Bebbington, 2001).

Assurance practice has emerged as a critical complement to disclosure, with cross-jurisdictional analyses documenting the heterogeneity of assurance standards, provider types, and engagement scopes that characterise the global market for sustainability assurance (Simnett, Vanstraelen & Chua, 2009). The determinants of voluntary assurance adoption further suggest that firms in stakeholder-oriented institutional environments and in industries facing higher reputational scrutiny are more likely to commission third-party verification, although the substantive rigour of such engagements varies considerably (Kolk & Perego, 2010). These observations imply that the value of an inventory cannot be assessed in isolation from the verification regime within which it is consumed, and that methodological frameworks must be designed with the assurance encounter explicitly in view.

A further conceptual dimension concerns the relationship between corporate inventories and life cycle perspectives on environmental impact. The life cycle approach, developed extensively in environmental engineering and industrial ecology, emphasises that the impacts associated with a product or service extend across multiple stages and across multiple actors, and that any apportionment among them involves ethical as well as technical considerations (Hertwich, 2005). The proposal to share producer and consumer responsibility, allocating emissions partly to those who manufacture and partly to those who ultimately consume, addresses the boundary problems of conventional accounting but introduces additional complications for the firm seeking to disclose a single, defensible footprint (Lenzen et al., 2007). Methodological debates within life cycle assessment have further raised the question of whether attributional approaches, which describe the inventory of a product as it currently is, can adequately support claims about mitigation outcomes, which are inherently consequential (Plevin, Delucchi & Creutzig, 2014).

The cumulative implication of these regulatory and conceptual developments is that the corporate inventory cannot be treated as a purely technical artefact awaiting standardised computation. It is instead a socio-technical construction whose credibility depends on the alignment of measurement procedures, reporting conventions, and assurance expectations. The methodological framework developed in this paper is designed to operate within this construction, harnessing the deterministic capabilities of process simulation while remaining attentive to the institutional logics of disclosure and verification. By making the engineering basis of the inventory transparent and traceable, the framework aspires to render the resulting figures simultaneously more accurate and more legible to the heterogeneous audiences that consume them.

A further consideration that distinguishes the contemporary regulatory environment from earlier reporting regimes is the increasing convergence between voluntary disclosure frameworks and mandatory regulatory schemes, which has elevated the evidential standards demanded of organisational inventories. Mandatory cap-and-trade schemes, mandatory disclosure rules in select jurisdictions, and the gradual incorporation of climate-related financial disclosure into mainstream corporate reporting have collectively raised the stakes attached to the methodological choices embedded in inventory construction. Whereas earlier voluntary reporting could tolerate considerable methodological latitude, the contemporary environment penalises ambiguity through both regulatory enforcement and reputational mechanisms operating through capital markets. This shift compels organisations to construct inventories that are not merely internally consistent but externally defensible, capable of withstanding adversarial scrutiny by regulators, auditors, and well-resourced civil society analysts whose claims-testing capacity has grown substantially.

The intersection of these regulatory pressures with the operational realities of energy-intensive process industries produces a distinctive set of methodological imperatives that any credible framework must address. Among these imperatives are the need for granular characterisation of fuel composition variability, the requirement to allocate emissions across co-products and co-generated energy outputs in a manner that survives external review, the necessity of treating fugitive and process-related emissions with rigour comparable to that applied to combustion sources, and the obligation to document the transition between historically reported and newly reformulated category structures with sufficient transparency to permit longitudinal comparability. The framework advanced in subsequent sections takes these imperatives as design constraints rather than as ancillary considerations, embedding them in the procedural architecture rather than addressing them through retrospective reconciliation.

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Equally important to the framing of organisational greenhouse gas accounting is the recognition that the inventory exists in dialogue with multiple regulatory and quasi-regulatory regimes that may impose distinct requirements on overlapping aspects of corporate performance. These include emissions trading scheme verification protocols, voluntary disclosure programmes administered by non-governmental institutions, sustainability indices used for institutional investment screening, and increasingly, the climate-related financial disclosure expectations of securities regulators. While each of these regimes has its own evidentiary conventions, they converge in their requirement that disclosed figures be supported by methodologically defensible computations whose underlying assumptions are documented and accessible. A simulation-grounded inventory framework satisfies these convergent requirements through a single coherent analytical infrastructure, reducing the duplication and inconsistency that arise when different reporting obligations are addressed through separate, narrowly tailored computations whose underlying assumptions may diverge in ways that are difficult to detect or reconcile.

III. PROCESS SIMULATION AS A FOUNDATION FOR INVENTORY CONSTRUCTION

The decision to ground a corporate inventory in process simulation rests upon the recognition that thermochemical installations are governed by conservation laws that admit, in principle, no exceptions: every kilogram of carbon entering the plant must leave it, and every joule of energy supplied must either be recovered, dissipated, or embodied in product transformations. The systematic exposition of plant design and synthesis demonstrates that mass and energy balances, far from being abstract pedagogical devices, constitute the indispensable scaffolding upon which any quantitative description of plant performance must be erected (Seider et al., 2009). When these balances are constructed at the level of the individual unit operation and then connected through stream relationships to form a flowsheet, the resulting model affords a depth of resolution that greatly exceeds what continuous emission monitoring or fuel meter aggregation alone can provide.

The economic and operational rationale for plant simulation has been further articulated through detailed treatments of plant design that integrate process synthesis, equipment sizing, utility integration, and economic evaluation into a single analytical framework (Towler & Sinnott, 2008). These treatments emphasise that the simulator's value is realised when it is calibrated against actual plant data, with model parameters adjusted iteratively until the predicted streams reproduce measured flows, compositions, and temperatures within acceptable tolerances. The calibrated model then serves as a reliable surrogate for the plant itself, capable of supporting both retrospective inventory construction and prospective scenario analysis.

The methodological lineage of material flow analysis provides an additional theoretical foundation for the simulation-based inventory. The systematic accounting of materials entering, accumulating in, and leaving a defined system, with attention to the quality and uncertainty of each flow, supplies the conceptual machinery through which simulator outputs can be aggregated to the organisational level (Brunner & Rechberger, 2004). When the boundaries of the material flow analysis are aligned with the consolidation choices made under the corporate inventory standard, a continuous accounting chain is established from the molecular composition of feedstocks to the kilograms of carbon dioxide equivalent reported in the firm's annual disclosure.

The integration of life cycle assessment with process optimisation has been an active area of inquiry for over two decades. Early work demonstrated that environmental performance metrics could be incorporated into process design alongside conventional economic objectives, with simulation tools providing the underlying mass and energy data (Azapagic & Clift, 1999). Subsequent contributions extended the approach to chemical processes more broadly, illustrating how simulator outputs could be coupled with characterisation factors to compute environmental indicators that informed both design choices and reporting (Burgess & Brennan, 2001). More recent work has refined these approaches by addressing the methodological challenges of multi-objective optimisation when life cycle considerations are introduced (Pieragostini, Mussati & Aguirre, 2012).

Sector-specific applications of these principles have generated rich evidence of their value. The cement industry, characterised by the dual emissions associated with limestone calcination and fuel combustion, has been the subject of extensive simulation-informed analysis. Foundational work documented the magnitude of cement-sector emissions and identified the process pathways through which they could be reduced, providing a quantitative anchor for subsequent inventory practice (Worrell et al., 2001). Process modifications, including the partial substitution of clinker by supplementary cementitious materials, have been evaluated through detailed engineering analyses that quantify their consequences for both the inventory and the product's mechanical performance (Habert et al., 2010). Critical reviews of energy use in the cement industry have catalogued the principal consumption points and the magnitudes of saving potential associated with various retrofits, supplying the kind of disaggregated data that simulator-based inventories require (Madlool et al., 2011). Surveys of emerging energy-efficiency and emission-reduction technologies have similarly emphasised that credible attribution of mitigation effects depends on baseline inventories grounded in plant-level engineering analysis (Hasanbeigi, Price & Lin, 2012).

The integrated steel sector exhibits comparable opportunities for simulation-grounded inventory construction. The chain of unit operations from sintering through coking, blast furnace ironmaking, and basic oxygen steelmaking is characterised by complex energy and materials integration, including the recovery and combustion of by-product gases that complicate the apportionment of emissions among process steps. Recent comprehensive reviews have documented progress on ultra-low carbon dioxide steelmaking pathways and have emphasised that the assessment of these pathways requires inventory frameworks capable of resolving the energy and material exchanges among integrated process units (Quader et al., 2016).

The implications of these developments for the construction of organisational inventories are substantial. A simulation-based approach permits the analyst to identify, for each unit operation, the precise carbon-bearing streams entering and leaving, the thermodynamic state of those streams, the conversions occurring within the unit, and the energy demands and recoveries associated with operation. From this resolved description, emission flows can be computed by elementary stoichiometric calculations, and energy demands can be traced to specific fuel and electricity inputs. The resulting inventory possesses a granularity and traceability that conventional approaches struggle to achieve, and the simulator file itself becomes the documentary evidence underpinning the disclosed numbers, available for inspection by verifiers and revisable as plant configurations evolve. This evidential function transforms simulation from a design aid into the central artefact of audit-ready disclosure.

The pedagogical and methodological foundations supporting this transformation merit closer examination, particularly because the disciplines of process systems engineering and corporate sustainability accounting have historically operated in relative isolation from one another, with each developing distinct vocabularies, evidentiary norms, and communication conventions. The simulation-based approach to inventory construction requires a substantive translation between these communities, in which thermodynamic and reaction-engineering concepts must be rendered intelligible to verifiers trained primarily in accounting and audit, while sustainability-reporting categories must be made operational for engineers accustomed to thinking in terms of mass flows and unit operations. The success of this translation depends not only on the technical adequacy of the simulator outputs but also on the development of documentation conventions that mediate between the two communities, providing audit trails sufficiently detailed to satisfy engineering rigour while sufficiently structured to satisfy verification protocols.

A complementary consideration is the temporal dimension of simulation-based inventory construction. The reporting period over which an organisational inventory is constructed typically spans a calendar or fiscal year, during which the plant will exhibit operational variability arising from feedstock fluctuations, demand-driven throughput changes, scheduled maintenance, and unplanned upsets. Capturing this variability within a single steady-state simulation requires the careful selection of representative operating points, the documentation of weighting rules used to aggregate them, and the systematic exclusion or inclusion of off-design conditions according to their materiality. The framework treats this temporal aggregation as an integral component of the simulation step rather than as a peripheral consideration, recognising that the credibility of the resulting inventory depends critically on the defensibility of the temporal averaging procedure.

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The case for simulation-based inventory construction is reinforced when one considers the alternative practices that simulation-based methods displace. Conventional approaches typically rely on aggregated fuel consumption data drawn from procurement records or utility billing, multiplied by tabulated emission factors selected from regulatory annexes or default databases. Such approaches discard the granularity that distinguishes one combustion configuration from another, attribute identical emissions to fuels of substantially different composition, and provide no mechanism for resolving anomalies between reported quantities and physically expected outcomes. The simulation-based alternative addresses each of these limitations by reconstructing the underlying physical processes with sufficient resolution to expose discrepancies between expected and observed performance, thereby supporting both more accurate disclosure and more reliable identification of opportunities for operational improvement. The methodological case for simulation is therefore not merely the absence of obvious deficiencies in the alternative but the active superiority of simulation-grounded analysis in producing inventories that meet the evidentiary expectations of contemporary disclosure regimes.

IV. METHODOLOGICAL ARCHITECTURE FOR BRIDGING SIMULATION AND INVENTORY

The methodological architecture proposed in this study comprises four sequential stages, each producing artefacts that feed forward into the subsequent stage and each generating documentary evidence amenable to third-party scrutiny. The first stage is boundary delineation, in which the reporting organisation determines the operational and equity perimeters of the inventory and selects a consolidation approach consistent with its corporate structure. Studies of the European cement industry have demonstrated that even within a single sector, choices about the inclusion of captive power plants, materials handling facilities, and ancillary operations can produce inventory differences of several percentage points, underscoring the materiality of boundary decisions (Pardo, Moya & Mercier, 2011). For each facility within the consolidation perimeter, the analyst then enumerates the unit operations that fall within scope and identifies the streams crossing the facility boundary, distinguishing those bearing combustion emissions from those bearing process emissions and from those representing imported energy.

The second stage is calibrated simulation, in which a steady-state model of each in-scope facility is constructed using a recognised process simulator and is parameterised to reproduce measured plant performance over the reporting period. Reviews of cement-sector emissions have shown that capturing the chemical reactions associated with calcination requires explicit treatment of the carbonate decomposition reaction, while combustion-related emissions depend on detailed fuel composition data and on the configuration of the kiln and preheater train (Ali, Saidur & Hossain, 2011). Strategic analyses of mitigation potentials in the same sector have similarly emphasised the importance of resolving alternative fuel substitution scenarios, since the substitution of waste-derived fuels for primary fossil fuels alters both the emission factor and the operational stability of the kiln (Benhelal et al., 2013). The simulator's role is to integrate these chemical and combustion phenomena into a coherent representation that respects conservation of mass and energy.

The calibration procedure proceeds by adjusting model parameters within physically defensible ranges until predicted flows, temperatures, and compositions reproduce measured values within tolerances determined by instrument accuracy and process variability. Where the plant is equipped with continuous monitoring of representative streams, calibration draws on these data; where direct measurement is unavailable, periodic laboratory analyses and engineering correlations supply the calibration anchors. The completed simulation produces a digital representation of the plant during the reporting period, from which the carbon flows associated with combustion and process reactions can be directly extracted.

The third stage is the translation of simulator outputs into inventory line items. For combustion sources, the analyst extracts the mass flow and composition of each fuel and applies stoichiometric carbon balances to compute the associated carbon dioxide emissions, with corrections for incomplete combustion where applicable and with separate accounting of methane and nitrous oxide derived from emission factors specific to the combustion technology and fuel type.

The decomposition of the energy system into its constituent flows has been extensively studied through global mappings of fuel-to-service energy chains, which provide a conceptual template for the translation step (Cullen & Allwood, 2010). For process emissions, the analyst applies stoichiometric relations to the relevant chemical reactions, drawing emission factors from the simulator's reaction network rather than from generic tabulations. This approach implements at the firm level the kind of disaggregated emission accounting envisioned in macro-economic studies of industrial decarbonisation potentials (Allwood, Cullen & Milford, 2010).

For imported energy, the calculation distinguishes between purchased electricity and purchased thermal energy, with each treated under both location-based and market-based reporting conventions, where the standard requires dual disclosure. Sectoral assessments such as those undertaken for the steel industry have emphasised the importance of separating energy carriers and accounting for their distinct emission intensities (Birat, 2010). The treatment of internal energy circulation, including the use of by-product gases recovered from coke ovens and blast furnaces, requires careful application of the operational control principle and benefits from the kind of materials-flow framework employed in studies of the global steel cycle (Pauliuk et al., 2013).

The fourth stage is uncertainty propagation, in which the analytical pipeline is extended to characterise the joint uncertainty associated with input data, model parameters, and emission factors, producing not only a point estimate of the inventory but also a quantified expression of its reliability. The aggregate evidence on industrial energy efficiency demonstrates that emission intensities can vary substantially with operational conditions, justifying the explicit treatment of variability rather than the assumption of fixed factors (Worrell et al., 2009). The economic literature on energy markets and management further emphasises that the boundary between operational variability and structural change is rarely crisp, and that the analytical framework must accommodate both temporal fluctuations and longer-term trends (Bhattacharyya, 2011). Engineering studies of motor systems and other auxiliary loads have shown that even within a stable operational regime, performance variability in support equipment can introduce non-trivial uncertainty into facility-level energy accounting, reinforcing the case for systematic propagation of parameter uncertainty through the simulation chain (McKane & Hasanbeigi, 2011).

The integration of these four stages into a coherent procedural pipeline yields several emergent benefits beyond the technical adequacy of the resulting numbers. The pipeline imposes discipline on data acquisition, since the calibration step exposes inadequacies in plant instrumentation that might otherwise remain hidden behind unverified manual data entries. It clarifies the division of analytical labour, since each stage produces well-defined deliverables that can be assigned to appropriately specialised personnel and then handed off through documented interfaces. It also produces a documentary trail amenable to incremental refinement, since improvements at any stage propagate forward to the disclosed numbers without requiring the wholesale reconstruction of the inventory. These procedural virtues are particularly valuable in organisations where inventory construction has historically relied on bespoke spreadsheet computations whose internal logic is opaque even to their authors after the passage of time.

A further design consideration in the methodological architecture is the explicit accommodation of organisational change. Energy-intensive process facilities undergo periodic capital investments, debottlenecking projects, fuel switching, and process modifications that alter the underlying mass and energy balances. The pipeline is designed so that such changes are reflected through controlled updates to the simulation model rather than through ad hoc adjustments to disclosed figures, with each update accompanied by documentation of the engineering rationale and by a parallel update to the uncertainty characterisation. This treatment of change as an ongoing feature of the inventory construction process, rather than as an exceptional disturbance, aligns the framework with the operational realities of plant management and supports the longitudinal comparability that disclosure standards increasingly demand.

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The four-stage architecture also accommodates the heterogeneity of facilities within multi-site organisations, where different plants may operate at different levels of process complexity, instrumentation maturity, and reporting consequence. The framework permits a tiered application in which the most material facilities receive the most rigorous simulation-based treatment while less material facilities are addressed through simplified mass-balance computations whose results are nevertheless reconciled with the corporate aggregate through the same procedural pipeline. This proportionality enables organisations to deploy analytical resources where they yield the greatest improvement in inventory quality, while preserving the methodological coherence of the consolidated disclosure. The capacity to differentiate analytical depth according to facility materiality is, in itself, a substantive contribution of the simulation-based approach, since alternative methods that apply uniform default factors across heterogeneous facilities cannot exploit the latent information that detailed analysis would surface for the most consequential operations.

V. DATA QUALITY, UNCERTAINTY QUANTIFICATION, AND AUDITABILITY

The defensibility of a simulation-based inventory hinges critically on the systematic management of data quality and on the rigorous propagation of uncertainty through the computational chain. Comparative methodological work on error propagation in environmental analyses has demonstrated that analytical, sampling, and Monte Carlo approaches each have characteristic strengths and limitations, with the choice among them depending on the structure of the inventory model, the distributional assumptions associated with the input parameters, and the computational resources available (Heijungs & Lenzen, 2014). For the simulation-based inventory, where the underlying engineering model is typically nonlinear and where input distributions may be skewed or correlated, sampling-based approaches offer particular advantages because they impose no linearity assumptions and naturally accommodate dependencies among parameters.

The categorisation of uncertainty in life cycle inventory has matured over the past two decades into a structured framework distinguishing parameter, model, and scenario uncertainties, with each requiring distinct treatment and with each contributing differently to the total uncertainty of the reported figure (Lloyd & Ries, 2007). For the corporate inventory, parameter uncertainty arises from the imprecision of measurement instruments, the variability of fuel composition, and the calibration tolerance of the simulator; model uncertainty arises from simplifications in the representation of unit operations and from approximations in the underlying thermodynamic and kinetic relations; scenario uncertainty arises from choices about temporal aggregation, allocation rules, and the treatment of atypical operating events. Studies of unresolved problems in life cycle assessment have argued that interpretive choices in impact assessment and characterisation can themselves generate substantial variability in reported results, an observation that translates to the corporate inventory as the choice among competing emission factor sources and global warming potential horizons (Reap et al., 2008).

The construction of high-quality background datasets has been a sustained focus of life cycle inventory research, with comprehensive databases providing emission factors for hundreds of energy carriers and material flows under harmonised methodological conventions (Hischier et al., 2010). The methodological framework underpinning these databases emphasises traceability, documentation, and the explicit characterisation of uncertainty for each entry, providing a model that simulation-based corporate inventories can productively emulate (Frischknecht et al., 2005). When the firm draws upon such databases for emission factors associated with imported energy or with raw materials whose upstream supply chains lie outside the simulator's boundaries, the inherited uncertainty must be propagated through the inventory calculation rather than discarded as background noise.

Best-practice guidance on characterisation modelling in environmental impact assessment has emphasised that the choice of characterisation factors and the treatment of regional and temporal differentiation can materially influence reported impacts, and that transparency about these choices is essential for credibility (Hauschild et al., 2013). For the corporate inventory, the analogue is the explicit documentation of the global warming potential metric employed, the time horizon over which it is computed, and the treatment of non-CO2 species whose climate impacts are particularly horizon-sensitive. The literature on impact assessment research has further argued that the boundary between methodological choice and value judgement is often porous, and that defensible reporting must surface the choices that have been made rather than embed them in implicit defaults (Bare, 2010).

The treatment of methodological choices in life cycle assessment has been comprehensively reviewed, with particular attention to the implications of system boundary selection, allocation rules, and end-of-life accounting for reported results (Finnveden et al., 2009). The corporate inventory faces analogous decisions, including the treatment of carbon credits and offsets, the allocation of emissions among co-products of integrated facilities, and the accounting for biogenic carbon flows. Each of these decisions must be documented with sufficient detail to permit reproduction of the inventory by an independent analyst working from the same source data, a standard that simulation-based approaches are well-positioned to meet because the simulator file itself constitutes a precise specification of all process assumptions.

The role of continuous emission monitoring deserves particular attention because it offers a measurement-based check on the simulation outputs and because it is increasingly required by environmental regulations applicable to large industrial sources. The technical literature on continuous monitoring has detailed the principles, configurations, calibration procedures, and quality assurance protocols associated with these systems, providing a foundation upon which the integration of measured and simulated data can be constructed (Jahnke, 2000). When measured concentrations and stack flows are available for representative emission points, they constitute an independent verification of the simulator's predictions and permit reconciliation of discrepancies through targeted re-examination of model parameters.

The institutional context of energy efficiency regulation provides additional drivers for the adoption of rigorous data quality practices. Reviews of policies and measures in the industrial sector have shown that mandatory reporting, voluntary agreements, and economic instruments each create distinct evidentiary requirements, with the most demanding regulatory regimes requiring monitoring, reporting, and verification practices comparable to those applied in financial reporting (Tanaka, 2011).

The simulation-based inventory framework developed in this paper is congruent with these expectations, since the digital twin produced by calibrated simulation supplies a coherent and reproducible evidential base that can be presented in support of regulatory submissions, voluntary disclosures, and assurance engagements alike. The auditor or verifier, confronted with a simulation-based inventory, is offered a documentary trail extending from the meter and laboratory results through the calibrated simulator to the disclosed figure, with each link inspectable and revisable. This continuity is the practical realisation of audit-readiness.

Beyond the technical mechanics of uncertainty propagation lies a deeper epistemic question concerning the appropriate calibration of confidence in disclosed figures. The simulation-based framework is, by virtue of its grounding in conservation laws and calibrated parameters, capable of producing inventories whose internal consistency exceeds that of conventional approaches, but this internal consistency must not be conflated with absolute accuracy. The remaining uncertainty arises from sources that lie beyond the simulator's reach, including the precision of the underlying instrumentation, the representativeness of laboratory analyses, the accuracy of upstream emission factors for purchased inputs, and the appropriateness of the global warming potential metric chosen for aggregating multiple greenhouse gas species. Disclosing these residual uncertainties candidly, rather than presenting the inventory as a precise figure shorn of qualification, supports the integrity of the disclosure and is increasingly expected by sophisticated consumers of corporate environmental information.

The audit interface of the simulation-based framework also benefits from the maturation of digital tools that support the inspection, version control, and incremental refinement of process models. Modern simulators provide audit logs of parameter changes, scenario archives that preserve the configurations underlying past inventory submissions, and structured export formats that facilitate independent re-execution of the calculations by verifiers equipped with compatible software. These capabilities elevate the verifier's role from spot-checker of selected figures to inspector of the underlying engineering model, a transition that aligns the practice of greenhouse gas assurance with the auditing of complex financial systems and that promises substantial gains in the depth and reliability of assurance engagements over time.

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Data quality considerations extend, finally, to the human and organisational factors that govern the production of inventory inputs. The most carefully designed simulation framework can be undermined by deficiencies in the supporting practices, including poorly maintained instrumentation, inadequately calibrated laboratory equipment, irregular sampling protocols, and inconsistent record-keeping. The framework therefore presupposes a programme of data governance that establishes standards for instrument calibration, laboratory accreditation, sample handling, and record retention commensurate with the evidential weight that the resulting figures will be expected to bear. Organisations adopting the framework must accordingly treat data governance as an integral component of inventory practice rather than as a peripheral administrative concern, recognising that the credibility of the disclosed figures depends ultimately on the integrity of the data flows that feed the simulator. This integration of technical and governance considerations distinguishes the proposed framework from approaches that emphasise computational sophistication without commensurate attention to the upstream practices that determine input quality.

VI. IMPLEMENTATION PATHWAYS IN ENERGY-INTENSIVE PROCESS INDUSTRIES

The application of the simulation-grounded inventory framework to specific energy-intensive industries reveals both common procedural patterns and sector-specific complications that demand contextual judgement. The cement industry, owing to its dual emission origins and its substantial energy demand, has been subject to particularly intense methodological scrutiny. Industry-led roadmaps have synthesised the projected contribution of efficiency improvements, alternative fuels, clinker substitution, and carbon capture to long-run decarbonisation, providing a sectoral context within which firm-level inventories must be situated (Cembureau, 2013). Within the proposed framework, the cement plant is represented as a flowsheet comprising raw material preparation, kiln-preheater-precalciner combustion and calcination, clinker cooling, and finish grinding, with simulator outputs distinguishing combustion-derived from process-derived carbon dioxide and tracking thermal energy demand to its constituent fuels.

Integrated steelmaking presents a more elaborate flowsheet challenge, with the simulator required to represent the iron ore preparation, coking, blast furnace ironmaking, basic oxygen steelmaking, and hot rolling operations as a connected materials and energy network. The recovery and internal combustion of coke oven gas, blast furnace gas, and basic oxygen furnace gas means that direct emissions are distributed across the flowsheet in ways that conventional fuel-input accounting can obscure. Comprehensive reviews of carbon capture and storage have detailed the integration challenges associated with retrofitting capture units onto integrated steelworks and have provided the technological context within which mitigation scenarios constructed atop the inventory can be evaluated (Boot-Handford et al., 2014). More recent assessments have emphasised the urgency of developing capture pathways for industrial sources whose emissions are difficult to abate through electrification alone, with the inventory serving both as the baseline against which mitigation is measured and as the operational accounting framework within which captured carbon must be tracked (Bui et al., 2018).

Hydrocarbon refining and bulk petrochemicals constitute the third archetype, with their characteristic features including extensive on-site cogeneration, complex hydrogen networks, and the integration of multiple process units around a small number of distillation, conversion, and treating operations. The carbon utilisation pathway, in which captured carbon dioxide is fed back as a feedstock for chemical conversion or fuel synthesis, has emerged as both a mitigation option and an inventory complication, since the same molecule of carbon may appear as an emission of one facility and a feedstock of another (Mac Dowell et al., 2017). The simulation-based approach handles this complexity by representing the carbon flows explicitly within the flowsheet of each facility, with cross-boundary transfers documented through stream specifications that connect the inventories of the affected entities.

The techno-economic assessment of carbon capture and storage applied to specific energy-intensive sectors has provided detailed unit-cost data and has identified the configuration choices that most strongly influence both the cost and the inventory implications of capture deployment (Leeson et al., 2017). For the firm contemplating capture, the simulation-based inventory permits a coherent comparison between baseline and capture-equipped operation, since the same flowsheet can be reconfigured to include the capture unit and its energy demands, with all consequences for direct emissions, imported electricity, and process steam reflected automatically in the recomputed inventory.

The broader trajectory of net-zero industrial systems sketched in recent integrated assessments emphasises that decarbonisation will require simultaneous transformations in energy supply, materials choice, and process configuration, with no single pathway sufficient and with substantial sectoral heterogeneity (Davis et al., 2018). The implication for inventory practice is that frameworks must be capable of representing successive plant configurations as the firm evolves, supporting both retrospective reporting of actual operation and prospective scenario analysis of contemplated changes. Methodological reviews of carbon footprint applications in the built environment have demonstrated the value of consistent inventory frameworks across heterogeneous applications, illustrating how methodological coherence supports both intra-organisational comparability and external benchmarking (Fenner et al., 2018).

The adoption of simulation-based inventory practices is, additionally, intertwined with the evolution of business models in which environmental performance becomes a strategic asset. Studies of business models for sustainable innovation have argued that the integration of environmental considerations into core operations requires both the technical infrastructure for accurate measurement and the organisational capabilities to translate measurement into strategic action (Boons & Lüdeke-Freund, 2013). The simulation-based inventory provides the former, while its successful deployment depends on management decisions about resourcing, training, and inter-functional coordination.

The framework's relevance extends beyond the highly industrialised settings in which most carbon accounting scholarship has been generated. Research conducted within emerging economy academic institutions has explored the intersection of advanced engineering education and sustainability research, illustrating how local knowledge production can support the contextualisation of methodologies developed in high-income jurisdictions (Adamah et al., 2016). Investigations of the relationships among renewable energy adoption, sustainable development, and environmental justice in such settings have further emphasised that decarbonisation cannot be reduced to the application of imported templates, but must be sensitive to local infrastructural realities, regulatory capacities, and distributive concerns (Adeojo & Osinibi, 2016). The simulation-based inventory framework, by emphasising plant-level engineering analysis and by accommodating site-specific data and constraints, is naturally well-suited to such contextualised application, enabling firms in jurisdictions with developing reporting infrastructures to construct inventories whose credibility does not depend on the prior availability of mature data systems.

The cross-archetype lessons that emerge from the framework's comparative implementation are instructive. The cement archetype foregrounds the importance of resolving process emissions arising from non-combustion chemical conversions, illustrating that inventory frameworks lacking the capacity to differentiate between fuel-derived and feedstock-derived carbon dioxide systematically misrepresent both the magnitude and the abatement potential of sectoral emissions. The integrated steel archetype highlights the centrality of internal energy circulation through by-product gas networks, demonstrating that conventional fuel-input accounting can produce results that diverge materially from physically grounded balances when applied to facilities characterised by extensive internal energy recovery. The refining and petrochemical archetype emphasises the methodological consequences of carbon utilisation pathways and complex hydrogen networks, showing that inventory frameworks must accommodate carbon flows whose physical disposition is genuinely ambiguous between emission, recycling, and product embodiment.

Practical implementation across these archetypes requires the cultivation of organisational capabilities that extend beyond the technical mastery of simulation software. The firm seeking to deploy the framework must invest in the integration of plant historian data with laboratory analytical results, in the development of engineering personnel capable of constructing and maintaining calibrated models, and in the institutionalisation of routines through which model updates are reviewed, approved, and incorporated into successive reporting cycles. These organisational investments are non-trivial, and they may exceed the appetite of firms whose carbon disclosure obligations remain primarily compliance-driven rather than strategically motivated. The framework's value proposition is accordingly clearer for firms that anticipate intensifying disclosure expectations or that have identified climate-related performance as material to their competitive positioning, since such firms can amortise the implementation costs across an extended horizon of strategic application.

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Beyond the four principal archetypes considered in detail, the framework's logic extends naturally to other energy-intensive process industries that share the structural features of complex thermochemical operation, including aluminium smelting, glass manufacture, pulp and paper production, ammonia synthesis, and large-scale chemicals more generally. In each of these settings, the underlying logic of representing the facility as a flowsheet of unit operations connected by streams remains applicable, and the simulator can be configured to capture the chemistry, energy demands, and emission flows that characterise the specific process. The principal sectoral differences lie in the choice of unit operation models, the selection of thermodynamic property packages appropriate to the working fluids, and the identification of the most consequential sources of uncertainty, but these are tactical adaptations within a common methodological architecture rather than departures from the core framework. The transferability of the approach across sectors is, accordingly, one of its principal strengths, since it offers a consistent methodological grammar within which heterogeneous industries can construct inventories that are mutually comparable and collectively credible.

VII. IMPLICATIONS, CHALLENGES, AND FUTURE DIRECTIONS

The synthesis presented in the foregoing sections carries several implications that warrant explicit elaboration, beginning with the conceptual claim that the corporate inventory is best understood as an evidentiary artefact rather than as a number. The methodological framework advanced here reframes inventory production as the assembly of a documentary chain extending from instrument readings and laboratory analyses through calibrated simulation to disclosed figures, with each link inspectable and revisable. This reframing aligns the corporate inventory with the broader project of understanding the life cycle environmental consequences of consumption, since the same engineering analyses that support direct-emission accounting can be extended to characterise upstream and downstream flows when reliable supplier data become available (Hertwich, 2011).

A significant analytical implication concerns the relationship between organisational inventories and the carbon footprint scholarship that has matured around products and services. Carbon footprints computed at multiple scales, ranging from individual products through firms, sectors, and nations, have been shown to exhibit characteristic patterns of consistency and divergence depending on the methodologies employed, with the most credible assessments grounded in transparent boundary definitions and rigorous documentation (Peters, 2010). The simulation-based inventory at the firm level provides a building block from which product-level footprints can be constructed by allocation, and from which sectoral and macro-economic figures can be aggregated through input-output extensions. The methodological coherence within and across these scales is one of the principal benefits of simulator-grounded inventory practice.

The framework also illuminates the role of energy infrastructure in shaping the inventory landscape. In jurisdictions where electricity is generated predominantly from low-carbon sources, the distinction between Scope 1 and Scope 2 emissions carries different practical implications than in jurisdictions where the grid is fossil-fuel-dominant. Strategic analyses of renewable energy development in emerging economies have demonstrated that the policy choices governing grid composition exert profound influence on the carbon intensity of industrial operations, and that firms operating in such settings face inventory dynamics shaped by national energy strategy as much as by their own operational decisions (Sambo, 2009). Comprehensive considerations of energy and sustainable development in such settings have further documented that the realisation of low-carbon transitions depends on coordinated action across electricity supply, industrial restructuring, and demand-side management, with implications for the temporal evolution of corporate inventories that simulation-based frameworks are well-suited to capture (Oyedepo, 2012).

Several challenges remain that future research and practice must address. The first concerns the resource intensity of constructing and maintaining calibrated simulators for facilities that may not have been designed with simulation-readiness in mind. Many older plants operate without comprehensive process information systems, and the historical record of stream measurements may be incomplete or inconsistent. Constructing a simulator for such facilities requires investment in instrumentation upgrades, in laboratory analysis programmes, and in the engineering effort required for calibration, all of which raise questions about the proportionality of the methodological burden to the firm's reporting obligations.

A second challenge concerns the treatment of dynamic and transient phenomena that fall outside the steady-state representation underlying most simulators. Plant start-ups, shutdowns, upset conditions, and equipment maintenance generate emission signatures that may differ substantially from steady-state operation and that contribute disproportionately to total emissions when their frequency is high. Extending the framework to handle dynamic simulation or supplementing the steady-state model with parametric corrections for transient events represents a productive direction for further development.

A third challenge arises from the boundary between the Scope 1 and Scope 2 categories under conditions of cogeneration, district heating, and shared infrastructure. The methodological convention of treating exported electricity from cogeneration as a deduction from gross emissions, while internally consistent, can produce reported figures that vary substantially with small changes in operational dispatch. The simulation framework's ability to resolve cogeneration explicitly through the underlying mass and energy balance offers a principled basis for this allocation, but does not eliminate the underlying definitional ambiguity.

A fourth challenge concerns the integration of simulation-based inventories into the regulatory and assurance ecosystems that increasingly govern climate disclosure. While the simulator file is, in principle, an ideal evidentiary artefact, its consumption by verifiers and regulators requires both technical fluency that may not be widely distributed in the assurance profession and standardised conventions for documentation, version control, and validation that remain in early stages of development.

Future work should accordingly address the standardisation of simulation-based inventory documentation in formats accessible to non-specialist reviewers, possibly through the development of structured exchange formats and audit checklists.

A fifth challenge concerns the treatment of value-chain emissions, which the present framework deliberately brackets but which the broader trajectory of corporate disclosure increasingly demands. Although simulation-based methods cannot, on their own, supply the supplier-specific data required for rigorous value-chain accounting, they can contribute to such accounting by providing the simulator-derived intensities for the firm's own outputs, which then become inputs into downstream customers' inventories. Building the institutional infrastructure to share such intensities reliably across supply chains, while protecting commercially sensitive information, represents a substantial agenda for both research and standardisation. Beyond the corporate scale, the broader credibility of comparative analyses that shape global understanding of industrial carbon flows ultimately rests on the methodological rigour of the firm-level inventories that feed them, reinforcing the case for treating simulation-based reporting as a foundational rather than peripheral element of the disclosure infrastructure.

A sixth and increasingly salient challenge arises from the rapid evolution of disclosure expectations under climate-related financial reporting initiatives, which are progressively transforming greenhouse gas inventories from peripheral environmental disclosures into integrated components of mainstream corporate reporting consumed by investors, lenders, and rating agencies. The simulation-based framework is well-suited to this elevated reporting context because it produces inventories accompanied by transparent methodological documentation and quantified uncertainty, satisfying the evidential expectations of financial-grade reporting more readily than approaches built on undocumented spreadsheet computation. The integration of greenhouse gas inventories into financial reporting also raises questions about materiality thresholds, restatement policies, and the treatment of prior-period adjustments, all of which the framework can accommodate provided that the underlying simulation models are version-controlled and that the documentation of methodological changes is maintained at a standard comparable to that applied in financial accounting.

Future research should additionally explore the integration of simulation-based inventories with adjacent analytical frameworks that share the methodological commitment to engineering rigour, including life cycle assessment, materials flow analysis, and techno-economic assessment. The conceptual and computational compatibilities among these frameworks suggest that a unified analytical platform supporting all of them simultaneously is technically feasible and would generate substantial efficiencies for organisations that currently maintain parallel modelling efforts in support of distinct reporting and analytical purposes. The development of such platforms, the articulation of the documentation conventions that govern their outputs, and the cultivation of the cross-disciplinary expertise required to operate them constitute an agenda whose pursuit promises to strengthen not only the practice of corporate carbon accounting but the broader project of evidence-based industrial environmental management.

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A final implication concerns the broader epistemic culture within which corporate climate disclosure is consumed. Recent decades have witnessed sustained debate about the credibility of corporate environmental claims, with episodes of greenwashing, methodological obfuscation, and selective disclosure undermining trust in the broader project. The simulation-based framework, by virtue of its commitment to documentary transparency and its anchoring in conservation laws, contributes to the rebuilding of that trust by offering disclosures that are inspectable, contestable, and improvable rather than opaque pronouncements demanding unconditional acceptance. The cultural shift required to consolidate this trust extends beyond the technical adequacy of any particular framework, but the framework's design embodies the disposition of openness and accountability that such a cultural shift requires. In an environment of intensifying public scrutiny and tightening regulatory expectations, this disposition is not merely an analytical preference but a strategic imperative, and the simulation-based approach offers organisations a credible response to that imperative that aligns engineering rigour with the demands of contemporary disclosure practice.

VIII. CONCLUSION

The architecture developed across the preceding sections offers a structured response to the persistent tension between the engineering reality of complex thermochemical installations and the disclosure-oriented logic of contemporary climate accounting. By grounding the construction of organisational greenhouse gas figures in calibrated process simulation, the approach treats conservation laws as the primary source of evidential authority and treats the simulator file as the central artefact of the documentary chain that ultimately supports independent verification. The four-stage pipeline encompassing boundary delineation, simulation calibration, output translation, and uncertainty propagation provides a transferable scaffolding within which sector-specific complications, including dual-origin emissions in cement, integrated by-product gas networks in steel, and elaborate cogeneration configurations in refining and petrochemicals, can be addressed coherently rather than through ad hoc workarounds. The framework's commitment to traceability between measured plant data and disclosed figures aligns it with the assurance expectations of mature jurisdictions while remaining adaptable to emerging-economy contexts where reporting infrastructures are still being constructed.

Several challenges await further work, particularly the extension of the steady-state core to encompass transient phenomena, the standardisation of simulator documentation for verifier consumption, and the integration of firm-level outputs into reliable value-chain accounting. Yet the conceptual gain is substantial: the inventory ceases to be an opaque computation and becomes a legible, contestable, and improvable engineering claim. For corporate sustainability practitioners, this transformation supplies a basis on which decarbonisation programmes can be designed and tracked with confidence; for regulators and verifiers, it offers a documentary substrate that withstands scrutiny; for the broader project of industrial climate governance, it suggests that the convergence of process systems engineering and corporate disclosure can yield reporting practices commensurate with the seriousness of the problem they address.

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