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ORIGINAL RESEARCH ARTICLE

Application chemistry-enabled precise allocation of carbon emission rights in the solar energy industry: Policy pathways and practical implementation models

Dandan Xie*

School of Business, University of Connecticut, 2100 Hillside Road, Unit 1041, Storrs, CT 06269-1041, USA

***Corresponding author:** Dandan Xie, dandan.xie@uconn.edu

ABSTRACT

The solar photovoltaic (PV) industry has been added to the decarbonisation plans for the world, but the manufacturing in its upper parts is still relatively high-carbon and difficult to quantify accurately. The present system of carbon emission allocation uses a single average emission factor or a historical intensity benchmark, thus failing to account for process and material-specific differences in reaction pathways. Application chemistry covers studies of reaction mechanisms, characterisation of new materials and high-throughput screening experiments to address the above deficiencies. Introduce a multi-scale framework in this paper to integrate molecular-level carbon tracing, process-level dynamic accounting and product-level carbon quota mapping to ensure the accuracy of carbon emission permit allocation for the solar energy industry. Three feasible policy-practice models for silicon production, photovoltaic cell fabrication and industrial chain integration have also been proposed. Based on the above analysis, it has been found that chemistry-informed carbon accounting can improve the accuracy of allocation and provide a direction for mechanism-driven design of the carbon market.

Keywords: application chemistry; photovoltaic industry; carbon emission rights; lifecycle carbon accounting; policy framework; carbon market design

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1. Introduction

To reduce the carbon emissions of the energy transition around the world, the first stage of solar PV module production must be carbon-free. Polysilicon production, wafer manufacturing and cell production are all high-temperature chemical reactions and energy-intensive processes that account for a large proportion of the carbon emissions in PV systems over their lifetime[1,2].

Emission factors and life cycle assessments (LCAs) are now used to calculate carbon accounting values, but they are relatively statistical in nature. They assume a uniform process and do not consider changes in the pathway of chemical reaction or material system. As a result, carbon allocation is often coarse-grained and does not fully reflect actual production structures; therefore, carbon pricing has lower precision and has reduced the incentive for technological optimisation.

Application chemistry can address the above problems by showing how carbon emissions arise in certain chemical reactions, material changes and energy-intensive processes. Based on reaction kinetics, thermodynamics and other high-end analysis equipment are used to identify the sources of emissions at the reaction stage, and they are no longer considered general outputs[3-5]. Although computational chemistry and data-driven methods have achieved good results in correlating process conditions with carbon intensity, research at the chemical level and in practice with carbon policy application still needs to be strengthened; currently, the carbon trading system does not include reaction-specific or material-specific emission data.

Therefore, this paper proposes a chemistry-based framework for precise carbon emission allocation in the PV industry and hopes to connect molecular-level reaction mechanisms with carbon policy design to construct an accurate and adaptable carbon accounting system.

2. Chemistry-based carbon accounting methodology

2.1. Limitations of conventional carbon accounting

Carbon accounting in the photovoltaic (PV) industry has traditionally used the emission factor method recommended by the Intergovernmental Panel on Climate Change (IPCC) and life cycle assessment (LCA) techniques[6,7]. Based on the above framework, total carbon emissions are calculated by multiplying activity

$$E = \sum_i Q_i EF_i \tag{1}$$

E is the total carbon emissions; Qi is the activity data of process iii, such as electricity consumption, raw material input or production capacity; and EFi is the corresponding emission factor obtained from industrial statistics or life-cycle databases. It is simple and has a small amount of data, so it has been widely used for carbon inventories at the industrial and national levels[8].

A typical type of derivation for emission factors is the empirical attribution method; it fails to consider changes in nature. Therefore, the influence of reaction paths, catalyst performance, reaction conversion efficiency and material utilisation cannot be separately identified and are included in averaged emission factors. As the development of high-end chemical processes for photovoltaic production, static emission factors are no longer suitable indicators of the primary sources of carbon emissions. Therefore, a chemistry-oriented accounting system should be built to connect carbon emissions directly with chemical reactions in production.

2.2. Reaction-based carbon accounting framework

Carbon emissions under chemical reaction engineering include those from the conversion of carbon-containing species in a closed-reactor system. Therefore, the framework presented here is based on chemical reactions rather than industrial activities at the level of the basic accounting unit. A typical chemical reaction is shown below:

$$\sum_i v_i A_i \rightarrow \sum_j v_j B_j \tag{2}$$

the progress of reaction r is quantified by the reaction extent,

$$\xi_r = \frac{\Delta n_i}{v_i} \tag{3}$$

where Δn_i is the amount of reactant consumed (or product generated) and ν_i is the corresponding stoichiometric coefficient. The extent of the reaction shows how far the chemical conversion has been realised and can provide a reference for evaluating the level of carbon generation in a reaction[9,10].

The carbon contribution of each reaction is expressed as a reaction carbon intensity

$$C_r = \frac{m_{CO_2,r}}{\xi_r} \tag{4}$$

where mCO2, r is the equivalent carbon dioxide generated by reaction r, and Cr is thus the carbon emission per unit of reaction extent. The general emission factor covers all links in the production process; however, for a specific chemical reaction, this carbon intensity can be altered by adjusting factors such as the reaction path, catalyst system, operating conditions, etc., and conversion efficiency is also a factor that changes it.

Therefore, the total carbon emissions from the production process can be shown as

$$E = \sum_{r=1}^{N_r} C_r \xi_r \tag{5}$$

where Nr is the total number of chemical reactions in the production system. Equation (5) shows that the total carbon emissions are the sum of the carbon contributions from all individual reactions. Equation (5) is not a mathematical modification of Equation (1); this should be pointed out. It has built a new carbon accounting system and moved the boundary of accounting from process-level activities to reaction-level carbon emissions. Compared with the traditional emission factor approach, the new formula directly relates carbon emissions to reaction pathways and material-change processes to offer a more mechanistic explanation of carbon generation in photovoltaic manufacturing[11-13].

2.3. Multi-Scale carbon aggregation and dynamic carbon accounting

Industrial production generally has many process units, and each unit involves several coupled chemical reactions. Therefore, the carbon emissions of a particular process can be obtained by summing up the contributions of all the reactions in that process,

$$E_p = \sum_{r=1}^{N_p} C_r \xi_r \tag{6}$$

where Np is the number of reactions in process ppp. Then, all process-level emissions are aggregated to find the total carbon emissions of the manufacturing system,

$$E_{system} = \sum_{p=1}^{M} E_p = \sum_{p=1}^{M} \sum_{r=1}^{N_p} C_r \xi_r \tag{7}$$

where M is the total number of production processes. The above hierarchy will build a bottom-up carbon accounting system to link reaction-level carbon emissions with process-level and system-level emissions[14-16].

The intensity of carbon emissions from the process is not assumed to be uniform. It will be different in all the operating circumstances, reaction paths, catalyst performance and process efficiency. Thus, the reaction carbon intensity can be generally expressed as

$$C_r = f(T, P, \eta, \lambda, \cdots) \tag{8}$$

T and P are the reaction temperature and pressure, respectively; η is the reaction conversion efficiency, and λ includes other process-dependent factors that affect carbon generation. Therefore, the proposed framework can dynamically update reaction-level carbon intensity as manufacturing technology changes, and a chemistry-based, mechanism-oriented approach to carbon allocation and process optimisation can be employed for low-carbon decision-making in photovoltaic manufacturing.

3. Reaction kinetics-based carbon emission allocation model

Most of the times, the method to calculate carbon emissions relies on statistics for energy use, materials and production. Although the above methods are convenient for carbon footprint estimation, they generally treat industrial processes as black boxes and fail to consider the intrinsic contribution of chemical reactions. Industries that undergo complex reaction processes, such as the production of photovoltaic materials, emit carbon through the reaction path, reactant conversion efficiency and reaction mechanism. Therefore, adding reaction kinetics to the allocation of carbon emissions provides a more basic measure of carbon responsibility[14,15].

3.1. Identification of reaction-related carbon emission contributions

Photovoltaic manufacturing emissions of carbon are due to both energy consumption and chemical-conversion processes. The latter are carbon-reduction reactions, decomposition reactions and the formation of carbon-containing intermediates. Reaction emissions directly correspond to the consumption of reactants and the efficiency of the reaction.

The amount of carbon emissions from an individual's behaviour is shown as follows:

$$C_i = n_i \times M_C \times \alpha_i \tag{9}$$

Where Ci is the carbon emission contribution of reaction i, ni is the amount of carbon-containing reactants participating in reaction i, Mc is the molar mass of carbon, and αi is a correction factor related to the conversion efficiency and actual operating conditions of reaction i.

Add the reaction parameters to carbon accounting and then quantify the contribution of each reaction path. Thus, the carbon responsibility can be attributed to the actual process contribution rather than solely to production volume or energy consumption[1].

3.2. Integration of reaction kinetics and life cycle carbon accounting

To build an all-encompassing carbon allocation system, reaction-related emissions have been included in the life-cycle assessment (LCA). The two kinds of carbon emissions for a photovoltaic product are energy-related emissions and reaction-related emissions.

$$C_{total} = C_{energy} + C_{reaction} \tag{10}$$

Cenergy refers to the indirect emissions from electricity and fuel consumption, and Creaction is directly generated emissions due to chemical reactions.

The corresponding proportions of the different production links can be identified by:

$$\lambda_i = \frac{C_i}{\sum C_i} \tag{11}$$

where λi is the carbon contribution coefficient of process i.

Previously, most of the LCA studies have focused on emissions from energy use; now we will also consider chemical properties in the industrial process. Therefore, processes that have the same energy consumption but different reaction mechanisms can be identified by their actual carbon-generation paths.

3.3. Reaction kinetics-based carbon allocation strategy

Given both the proportion of reaction contribution and life-cycle carbon emissions, a reaction-kinetics-based carbon allocation method will be employed to determine the carbon responsibility of different production paths. Instead of dividing carbon emissions based on product mass, energy consumption or economic value, a new system will be introduced that assigns carbon responsibility according to how the actual emission is produced by chemical-transformation processes[7].

The process carbon allocation coefficient is the sum of the energy part and the reaction part:

$$\beta_i = w_1 \frac{C_{energy,i}}{\sum C_{energy,1}} + w_2 \frac{C_{reaction,i}}{\sum C_{reaction,i}} \tag{12}$$

where βi is the overall carbon contribution coefficient of process i, Cenergy,i and Creaction,i are the energy-related and reaction-related carbon emissions, respectively, and ω1 and ω2 are weighting factors that reflect the relative importance of energy consumption and reaction processes.

According to the calculated allocation coefficients, the total carbon emissions of all links in the production process are as follows:

$$A_i = \beta_i C_{total} \tag{13}$$

where Ai is the carbon allocation for process i.

Therefore, the firm will be held accountable for the source of emissions. Processes with inefficient reactions, excessive carbon consumption or unfavourable reaction pathways will be assigned a higher carbon liability; therefore, improving the efficiency of the reaction, enhancing reactant utilization and optimising the process can reduce this assigned carbon responsibility.

Thus, the new reaction kinetics-based allocation plan for carbon emissions provides more specific operating instructions. Improve the accuracy and fairness of carbon allocation, establish a quantitative link between technological innovation and emission reduction results, provide a theoretical foundation for carbon trading, emission regulation and the low-carbon development of the photovoltaic industry, etc.

4. Application of the reaction kinetics-based carbon allocation model in the photovoltaic industry

The different links in the production process of photovoltaic panels are raw material processing, silicon purification, wafer production, solar cell manufacturing and module assembly. The Carbon Footprint of photovoltaic products is relatively sensitive to both energy consumption and chemical-conversion processes. Therefore, to establish an effective carbon allocation system, we need to know the emissions at all links of production[1].

The proposed reaction kinetics-based carbon allocation model will be applied to the photovoltaic manufacturing chain in this section. Distribute the characteristics of carbon emissions and show that, through a new approach, the results can be improved over those of traditional allocation by considering reaction mechanisms in carbon responsibility assessment.

4.1. Carbon emission distribution across photovoltaic manufacturing processes

Most of the carbon emissions from the production of photovoltaic modules occur at the start of the process in China. Compared with the downstream processes of wafer cutting, cell fabrication and module assembly, silicon purification and preparation are high-temperature processes involving complex chemical reactions and high-energy consumption, thus contributing to more carbon emissions.

According to the new division plan, energy-related emissions and reaction-related emissions have been split. As a result, the carbon emissions from energy use are still relatively high due to the power-intensive nature of high-temperature processes. However, reaction-related emissions are also relatively large in some processes that use carbon-containing reducing agents or chemical-to-chemical conversion[12,17].

The old way of carbon accounting generally attributes emissions according to energy consumption or production volume; however, the new reaction kinetics-based model considers all reaction paths and conversion efficiencies to address this problem. For example, the two manufacturing processes have the same energy consumption but different carbon footprints due to different reaction mechanisms, reactant utilisation efficiencies and carbon conversion behaviours.

Thus, the above framework offers more detailed information on the sources and dissemination paths of carbon emissions in photovoltaic manufacturing.

4.2. Comparison between conventional and reaction kinetics-based carbon allocation methods

Traditionally, the indicators in carbon accounting have been relatively simple, such as production volume, energy consumption and economic value of the product. Although the above methods are practical for large-scale carbon inventories, they may not be suitable for attributing carbon emissions to specific processes with complex chemical transformations accurately.

A reaction kinetics-based model introduces reaction contribution factors in carbon allocation to provide a process-oriented assessment of carbon responsibility. Compared with the former way, the new method can determine whether the emission is due to low-efficiency energy use or inherent chemical conversion.

It is also required to reduce emissions in this way. To reduce carbon emissions from energy use, integrate renewable electricity, improve energy efficiency, and optimise the use of process heat. Reaction-related emissions need to be reduced by using carbon-free reagents, enhancing the selectivity and conversion rate of the reaction, or finding new reaction routes.

Therefore, the proposed model has converted carbon allocation from a fixed-accounting method into a dynamic-evaluation system that links emission responsibility with technological-improvement prospects.

4.3. Implications for low-carbon photovoltaic development and carbon policy

The application of the proposed model offers some references for the future low-carbon development of photovoltaic power generation. First, carbon allocation according to reaction mechanisms can improve the fairness of carbon responsibility distribution at different stages of production. Enterprises that improve the response efficiency or material-use technology of the company will reduce their carbon footprint in a tangible way.

Second, the model will provide a scientific basis for establishing carbon emission standards and constructing a carbon trading system. At present, most carbon management strategies use total emission inventories and fail to account for process differences. Add reaction contributions to allocate carbon allowances in line with the actual emission-generation path of industrial processes.

In addition, the proposed framework is not only for photovoltaic production. Other areas that may also be related to this type of chemical reaction include metallurgy, battery materials and semiconductor manufacturing, etc. Therefore, reaction kinetics-based carbon allocation offers a general way to combine basic chemical knowledge with industrial carbon management.

5. Conclusion

A reaction kinetics-based carbon emission allocation framework has been introduced in this paper to address the defects of the traditional carbon accounting method, which only uses statistical indicators such as energy consumption and product output. Add the natural contribution of chemical reaction processes in life-cycle carbon accounting to create a more process-oriented system for distributing carbon responsibilities in the photovoltaic industry. The first few are as follows:

(1) Based on reaction kinetics, separate accounting for energy-related and reaction-related carbon emissions was employed. The framework proposed will be able to determine the origin of carbon emissions from photovoltaic manufacturing more precisely by considering reaction paths, reactant consumption and conversion efficiency.

(2) A model of carbon emissions for reaction emissions and life-cycle emissions was built. Under the old system of dividing responsibility for carbon emissions based on production scale or energy consumption, it was unclear who was responsible; now, however, the exact reason for the emission is known and which link in the process accounts for this emission has been identified.

(3) The new system will be used in the photovoltaic industry to find carbon-intensive links in the process and formulate a reduction plan. Link carbon responsibility to technological improvements in energy efficiency, reaction optimisation and material utilisation to provide a scientific basis for carbon allowance allocation and low-carbon transformation.

In short, this paper demonstrates that the mechanism of a chemical reaction is required for industrial carbon management. A general path for energy- and material-intensive industries with complex chemical processes has been proposed by the reaction kinetics-based carbon allocation framework to promote higher-precision carbon accounting and green industrial development.

Conflict of interest

The author declares no conflict of interest.

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