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Constraint-aware online coarse-to-fine optimization of crystalline silicon photovoltaic devices

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Abstract

Designing crystalline-silicon photovoltaic devices requires exploration of coupled parameters under multiple electrical constraints. Here, we present a constraint-aware online coarse-to-fine optimization approach that integrates automated device generation, performance extraction, feasibility classification, and current-best tracking within a single PC1D-based simulation loop. A joint-sensitivity criterion selects variables strongly associated with open-circuit voltage, short-circuit current density, and fill factor. The method evaluates 100,243 configurations for a multilayer crystalline-silicon solar cell. A global coarse-grid search identifies a candidate design, and local high-resolution refinement yields a refined optimal configuration with 17.5249% efficiency while satisfying all imposed constraints. One-dimensional sweeps reveal feasible boundaries and parameter–performance trade-offs around the selected design. An independent reduced-grid SCAPS-1D exploration followed by constraint-enforced local refinement recovers the same refined design-variable settings, providing cross-solver numerical consistency. Compared with full-domain fine-grid scenarios, the coarse-to-fine approach substantially lowers the estimated computational burden. These results provide a transparent and practical route for simulation-driven photovoltaic-device optimization.

Keywords: Crystalline silicon solar cells; Constraint-aware optimization; Coarse-to-fine search; Joint-sensitivity analysis; Cross-solver consistency; Photovoltaic device simulation

I. Introduction

Solar photovoltaic technologies have become central to the global energy transition because of their scalability and rapidly expanding deployment potential [1], [2]. The continuing decline in renewable-electricity costs has further strengthened the role of photovoltaics in low-carbon energy systems [3], while global photovoltaic demand is expected to increase as power-sector decarbonization progresses [4], [5]. As deployment expands, further improvements in conversion efficiency, reliability, manufacturing feasibility, and development cost remain essential [6], [7]. Optimization of photovoltaic devices is therefore increasingly important for identifying high-performance configurations before fabrication [8]. Broader reviews of photovoltaic technologies also highlight the need for systematic design strategies capable of addressing coupled material, structural, and operating parameters [9], [10]. In this context, computational methods that can efficiently explore multivariable design spaces while enforcing practical performance requirements are needed to reduce the burden of pre-fabrication device design.

Crystalline-silicon solar cells remain the dominant photovoltaic technology because of their mature manufacturing infrastructure, long-term reliability, and continuously improving efficiency [11]. The evolution of photovoltaic-cell generations shows that silicon-based devices retain a central role despite the emergence of alternative materials and architectures [12]. Improvements in high-efficiency silicon solar cells require careful control of carrier generation, transport, recombination, and contact-related losses [13]. Manufacturing-oriented studies

further emphasize the importance of process compatibility and device robustness [14], while advanced architectures, surface passivation, and light-management strategies provide major routes towards improved performance [15]. Light-trapping structures have also been investigated to enhance photon absorption and carrier collection in thin silicon devices [16]. However, increasing structural complexity makes empirical trial-and-error design increasingly costly and difficult to generalize [17], [18]. Parameter-level PC1D studies have shown that doping concentration substantially affects crystalline-silicon device performance [19], and temperature-dependent investigations demonstrate that V_{oc} , J_{sc} , FF , and conversion efficiency vary with operating temperature [20], [21]. These coupled dependencies make systematic multivariable exploration necessary for reliable device optimization.

Physics-based device simulation provides an efficient route for evaluating photovoltaic structures before fabrication [22], [23]. Reliable cell modeling and parameter estimation are essential for meaningful performance prediction [24], [25], and comparisons of photovoltaic simulation tools demonstrate their value for investigating material properties, device geometry, and operating conditions [26]. PC1D has long been used as a one-dimensional semiconductor simulator for silicon solar-cell analysis [27]. The cmd-PC1D implementation introduced advanced crystalline-silicon models and command-line execution suitable for automated simulation [28], while PC1Dmod incorporated updated physical models within the established PC1D interface [27–29]. SCAPS-1D has similarly been applied to the analysis and optimization of layered photovoltaic structures [30], [31]. More generally, numerical studies and reviews show that physics-based simulations can support the exploration of complex photovoltaic design spaces and accelerate the identification of high-performance configurations [32], [33]. Nevertheless, increased simulation throughput alone does not determine how generated cases should be screened for feasibility, ranked during exploration, or selected for subsequent refinement.

Data-driven photovoltaic research has also expanded through open databases, large simulation datasets, and machine-learning-assisted analysis. Open photovoltaic databases provide structured resources for reproducible large-scale studies [34], and big-data analysis has revealed stability trends and performance-relevant relationships in photovoltaic datasets [35]. At the device level, SCAPS-assisted machine-learning studies have supported photovoltaic-parameter prediction and layer-level design [36], [37], while machine-learning analysis has been used to relate material properties to photovoltaic-device behavior [38]. Monte Carlo analysis has further shown that variability in modeling parameters can be correlated with photovoltaic performance [39]. More recently, neural-network-assisted device characterization using a 100,000-sample simulation dataset has been reported to accelerate parametric studies, sensitivity analysis, and optimization [40]. These studies demonstrate the value of large-scale numerical data, but they do not by themselves establish a unified process in which feasibility assessment, optimum tracking, local refinement, and independent solver comparison are connected during design-space exploration.

Related photovoltaic-optimization studies have demonstrated automated PC1D-based design-space exploration, feasibility filtering, objective-function evaluation, and SCAPS cross-simulation [41]. Multi-resolution optimization has also shown the effectiveness of global coarse-grid screening followed by local high-resolution refinement [42]. Building on these developments, further investigation is required to determine whether joint-sensitivity screening, case-wise online feasibility classification, current-best updating, local response analysis, and an independently executed SCAPS-1D coarse-to-fine search can be integrated within a single crystalline-silicon design study. Such integration is particularly relevant when design feasibility depends simultaneously on V_{oc} , J_{sc} , and FF , and when the selected configuration must be assessed against solver-specific numerical behavior. Reported crystalline-silicon studies provide physical and practical context for defining device-performance requirements and admissible design ranges [43]–[45].

Here, we present a constraint-aware online coarse-to-fine optimization approach for crystalline-silicon photovoltaic devices. A joint-sensitivity criterion is first used to retain parameters that exhibit consistently strong associations with V_{oc} , J_{sc} , and FF . The selected design space is then explored using an automated PC1D workflow in which each generated case is simulated, classified as feasible or infeasible, and compared with the current best feasible configuration during case generation. A global coarse-grid search is followed by local high-resolution refinement to identify the refined optimal configuration within the discretised feasible domain. Automated one-dimensional sweeps are used to interpret feasible boundaries and parameter–performance trade-offs around the selected design. An independent reduced-grid SCAPS-1D exploration followed by constraint-enforced local refinement is subsequently conducted to assess cross-solver numerical consistency. Finally, the computational burden of the proposed coarse-to-fine approach is compared with full-domain fine-grid search scenarios. Together, these analyses provide a transparent and practical route for simulation-driven crystalline-silicon photovoltaic-device optimization.

II. Methods

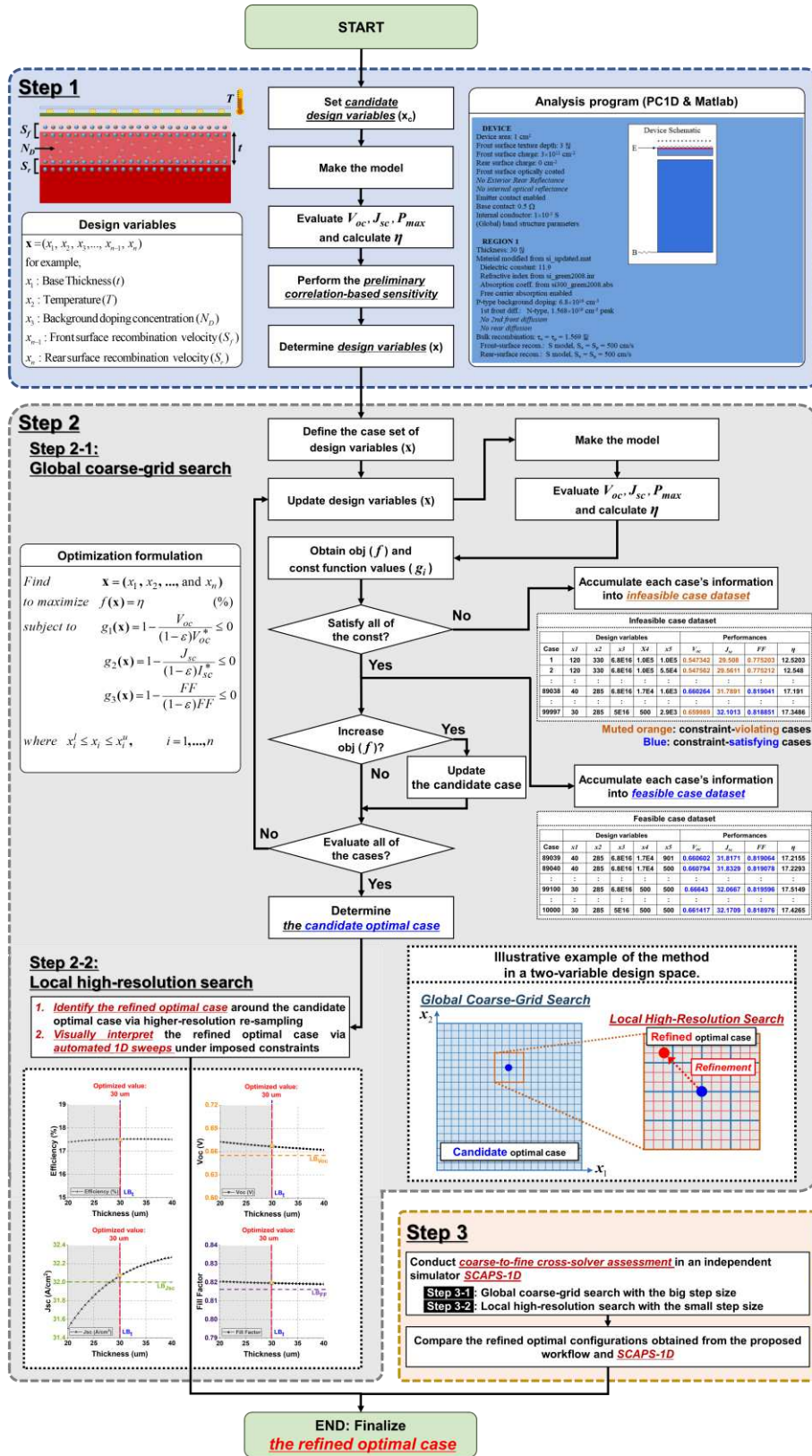


Figure 1. Overview of the proposed constraint-aware online coarse-to-fine optimization approach. Step 1 performs automated virtual-device construction and joint-sensitivity-guided selection of effective design variables. Step 2 evaluates each simulated case online, classifies feasible and infeasible cases, updates the current best feasible design, and identifies candidate and refined optimal configurations through PC1D-based coarse-to-fine exploration and one-dimensional sweep analysis. Step 3 independently performs a reduced-grid SCAPS-1D coarse exploration followed by constraint-enforced local refinement to assess cross-solver numerical consistency.

This section presents a constraint-aware online coarse-to-fine optimization approach for multilayer crystalline-silicon photovoltaic devices (Fig. 1). Unlike conventional workflows that first generate a complete dataset and subsequently perform feasibility screening and optimum selection as separate post-processing tasks, the proposed workflow integrates joint-sensitivity-guided variable selection, case-wise constraint evaluation, feasible–infeasible classification, and current-best tracking within an automated simulation process. A global coarse-grid exploration first identifies a candidate optimal case, which is subsequently refined through a local high-resolution search. Automated one-dimensional sweeps are then used to interpret the objective and constraint responses around the refined optimum. Finally, SCAPS-1D is used as an independent simulator to assess regional and refined-level numerical consistency with the PC1D-derived design configuration.

II-A. Step 1: Automated virtual-device construction and joint-sensitivity screening

In Step 1, the target solar cell is constructed in a virtual environment using an in-house automated framework that couples the open-source one-dimensional semiconductor device simulator PC1D with internally developed scripting and data-extraction modules. The automated workflow comprises design-variable assignment, device-model generation, simulation execution, and extraction of performance indicators from illuminated J–V characteristics. This automation maintains consistent numerical settings across the generated cases and eliminates repeated manual intervention. The baseline device-model parameters and simulation settings are provided in Supplementary Table S1.

Based on the generated simulation outputs, a preliminary correlation-based joint-sensitivity analysis is conducted to identify candidate parameters exhibiting consistently strong associations with all three key performance indicators. For each candidate parameter p , the joint-sensitivity score is defined as

$$S_p = \min \left(\left| r_{p,V_{oc}} \right|, \left| r_{p,J_{sc}} \right|, \left| r_{p,FF} \right| \right), \quad (1)$$

where $r_{p,V_{oc}}$, $r_{p,J_{sc}}$, and $r_{p,FF}$ denote the Pearson correlation coefficients between parameter p and the corresponding performance indicators. The absolute correlation magnitude is used for screening because the sign indicates the direction of the relationship, whereas the magnitude indicates its strength. In this study, an application-specific threshold of $S_p \geq 0.90$ is used. A candidate parameter is therefore retained as an effective design variable only when its absolute Pearson correlation coefficient is at least 0.90 for each of V_{oc} , J_{sc} , and FF . This joint-screening criterion reduces unnecessary dimensionality while preserving the variables that collectively govern voltage, current-density, and fill-factor responses. Further details of the one-factor-at-a-time sampling and Pearson-correlation procedure are provided under “OFAT sampling and Pearson-correlation procedure” in the Supplementary Information. The admissible ranges and sampling settings of the retained variables are provided in Supplementary Table S2 and are used in the Step 2 search.

II-B. Step 2: Constraint-aware online coarse-to-fine optimization

Step 2 comprises a global coarse-grid search followed by local high-resolution refinement. Using the effective design variables retained in Step 1, the global stage identifies the highest-efficiency feasible configuration at coarse resolution, hereafter termed the candidate optimal

case. The local stage then re-samples a narrow region around this candidate under the same electrical-performance constraints to identify the refined optimal case. The detailed global and local procedures are described in Steps 2-1 and 2-2, respectively.

For consistent case handling, each evaluated configuration is represented by its design variables, performance indicators, and feasibility status, while the current best feasible configuration is updated during case generation. The corresponding case representation and update rule are defined in Step 2-1.

II-B-1. Step 2-1: Global coarse-grid search and candidate optimal case identification

Step 2-1 uses a global coarse-grid search to systematically explore the predefined design space and identify the highest-efficiency feasible configuration at coarse resolution. All prescribed configurations are evaluated while the design-variable bounds and electrical-performance constraints are enforced.

The optimization problem is formulated as the following constrained maximization problem:

$$\begin{aligned}
& \text{Find} && \mathbf{x} \\
& \text{to maximize} && f(\mathbf{x}) \\
& \text{subject to} && g_i(\mathbf{x}) \leq 0 \quad i = 1, \dots, m \\
& && x_j^l \leq x_j \leq x_j^u \quad j = 1, \dots, n
\end{aligned} \tag{2}$$

where $\mathbf{x}$ is the vector of effective design variables retained in Step 1, $f(\mathbf{x}) = \eta(\mathbf{x})$ is the conversion-efficiency objective, $g_i(\mathbf{x})$ is the i th constraint function, and x_j^l and x_j^u denote the lower and upper bounds of the j th design variable, respectively. The application-specific forms of the constraint functions and their threshold values for the crystalline-silicon case study are specified in Section III-B-1.

Online case evaluation and current-best update rule

Each evaluated configuration k is represented as

$$C_k = (\mathbf{x}_k, \mathbf{y}_k, \delta_k), \tag{3}$$

where $\mathbf{x}_k$ is the design-variable vector, $\mathbf{y}_k = (V_{oc,k}, J_{sc,k}, FF_k, \eta_k)$ is the corresponding performance vector, and δ_k is the binary feasibility indicator:

$$\delta_k = \begin{cases} 1, & g_i(\mathbf{x}_k) \leq 0 \text{ for all } i = 1, \dots, m, \\ 0, & \text{otherwise} \end{cases} \tag{4}$$

Once the first feasible configuration is identified, the current best feasible design after k evaluations is updated as

$$\mathbf{x}_k^{\text{best}} \in \arg \max_{1 \leq j \leq k, \delta_j = 1} f(\mathbf{x}_j) \tag{5}$$

This formulation enables consistent case-wise feasibility classification and objective-based best-case updating during simulation. All prescribed cases are nevertheless evaluated; therefore, the online update rule does not introduce early stopping or reduce the number of PC1D simulations.

Unlike workflows in which feasibility screening and optimum selection are performed only after dataset generation, each coarse-grid case is processed sequentially during case generation. For each case, the device model is constructed, the performance indicators are extracted, the constraint functions are evaluated, and the feasibility indicator (δ_k) is assigned. Feasible cases ($\delta_k = 1$) are ranked according to $f(\mathbf{x}_k)$, and the current best feasible design $\mathbf{x}_k^{\text{best}}$ is updated according to Eq. (5). After all prescribed coarse-grid cases have been evaluated, the final current-best design is retained as the candidate optimal case without requiring a separate global post-processing step.

The candidate optimal case is used to define the local high-resolution search region in Step 2-2. The refined optimal case identified from that search is subsequently used as the reference configuration for the one-dimensional sweep analysis.

II-B-2. Step 2-2: Local high-resolution refinement and one-dimensional sweep analysis

In Step 2-2, local high-resolution refinement is conducted in the neighborhood of the candidate optimal case identified in Step 2-1. A finer discretization with smaller variable increments is used to characterize the local objective and constraint responses under the same feasibility requirements applied in the global search. The refined optimal case is defined as the highest-objective feasible configuration identified within the locally refined and discretized design space; the term does not imply a continuous-domain analytical global optimum.

During local re-sampling, the configurations within the refined region are generated and evaluated automatically. The same constraint-evaluation, feasibility-classification, and objective-ranking rules used in the global search are applied to all local configurations. The feasible configuration yielding the maximum objective value within the refined region is retained as the refined optimal case.

The local-refinement grid and the one-dimensional sweep datasets serve distinct but complementary purposes. The local grid covers a narrow region around the candidate optimal case and provides the quantitative basis for identifying the refined optimal case. In contrast, the one-dimensional sweeps are performed over broader, application-specific ranges around the refined optimal configuration. During each sweep, one retained design variable is varied while all remaining variables are fixed at their refined optimal values. The resulting profiles describe the objective response, constraint responses, feasible boundaries, and parameter–performance trade-offs as the design moves away from the selected configuration.

The one-dimensional sweeps are used for local-response interpretation rather than as an additional multidimensional optimization stage. They do not alter the refined optimal case identified from the local full-factorial grid. The application-specific local-refinement levels and one-dimensional sweep ranges are reported in Section III-B-2 and Supplementary Table S2.

II-C. Step 3: Independent SCAPS-1D coarse-to-fine cross-solver assessment

Step 3 uses an independent SCAPS-1D coarse exploration followed by constraint-enforced local refinement to assess numerical consistency with the PC1D-derived refined configuration. The same design-variable bounds, conversion-efficiency objective, and application-specific feasibility constraints used in Step 2 are retained. Unlike the automated PC1D workflow, the SCAPS-1D configurations are constructed and evaluated manually through the graphical user interface. The procedure comprises a reduced-resolution coarse exploration followed by local high-resolution refinement.

At the coarse level, the predefined design space is independently re-explored at reduced resolution. The highest-efficiency coarse configuration is selected as a high-performance reference case for subsequent local refinement. This configuration is used to locate an independently derived high-performance region and define the refinement center; it is not regarded as the final constraint-satisfying optimum. Accordingly, the SCAPS coarse stage does not adopt the PC1D-derived refined optimum as its starting point.

At the refined level, local high-resolution refinement is performed around the SCAPS-derived coarse reference case using smaller variable increments. The same conversion-efficiency objective and feasibility constraints are applied to all refined configurations. The highest-efficiency feasible configuration within the refined region is retained as the SCAPS-derived refined optimal case. Its design-variable settings are then compared with those of the PC1D-derived refined optimal case identified in Step 2-2.

Cross-solver consistency is assessed primarily by comparing the design-variable settings of the independently obtained PC1D and SCAPS refined optimal cases. Strict equality of V_{oc} , J_{sc} , FF , or conversion efficiency is not required because the two simulators use different numerical formulations, material databases, and boundary-condition treatments. Agreement in the selected refined design-variable configuration is interpreted as reducing the likelihood that the result is specific to a single simulator; it is not treated as experimental validation. The application-specific SCAPS grid settings and results are reported in Section III-C, while detailed paired PC1D–SCAPS performance values are provided in Table 5.

III. Application to a multilayer crystalline-silicon solar cell and results

This section presents the application of the proposed constraint-aware online coarse-to-fine optimization approach to a multilayer crystalline-silicon solar cell. Step 1 established the baseline device model and applied joint-sensitivity screening to identify the effective design variables. Step 2 applied the online coarse-to-fine search to identify the PC1D-derived refined optimal configuration and used one-dimensional sweeps to examine its local objective and constraint responses. Step 3 independently re-explored the design space using a reduced SCAPS-1D coarse grid, applied constraint-enforced local refinement around the resulting high-performance reference case, and compared the SCAPS-derived refined configuration with the PC1D-derived configuration. Steps 1 and 2 were executed automatically, whereas the SCAPS-1D cases were constructed and evaluated manually through the graphical user interface.

III-A. Step 1: Baseline device model and joint-sensitivity screening results

In Step 1, a multilayer p-type crystalline-silicon solar cell operating under standard AM1.5G one-sun illumination was selected as the application model. The device structure included the functional regions required to represent optical absorption, carrier transport, and bulk and surface recombination. The schematic structure and the locations of the five variables retained by joint-sensitivity screening are shown in Fig. 2.

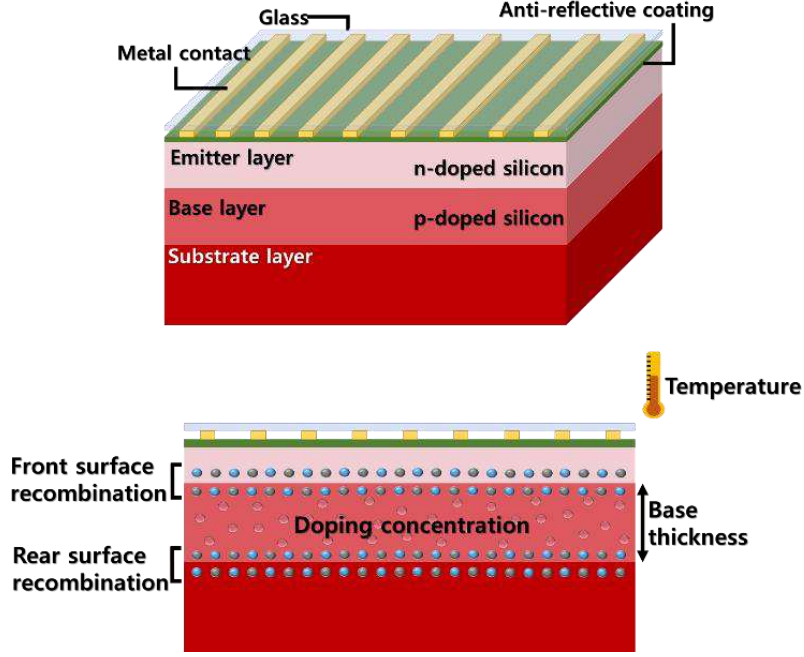


Figure 2. Schematic multilayer crystalline-silicon device structure used in the case study and the five variables retained by joint-sensitivity screening

The application model was implemented using the automated PC1D–in-house environment described in Section II-A. For each prescribed parameter set, the environment generated the corresponding device model, executed the simulation, and extracted V_{oc} , J_{sc} , FF , and conversion efficiency from the illuminated J – V characteristics. This automated execution maintained consistent numerical settings across all evaluated cases.

The baseline model represented a multilayer p-type crystalline-silicon solar cell under standard AM1.5G one-sun illumination. The layer sequence and the locations of the principal structural and electrical parameters are shown in Fig. 2. The principal baseline values are specified below, while the complete PC1D input set and numerical settings are provided in Supplementary Table S1. The baseline values were selected from published crystalline-silicon device studies and were representative of a conventional p-type c-Si solar-cell structure [44]. Unless otherwise specified, the simulations retained the PC1D models for Shockley–Read–Hall and Auger recombination, intrinsic carrier concentration, carrier mobility, and optical absorption. The illuminated J – V response of this baseline configuration was used as the reference state for subsequent parameter variations and performance evaluation. The baseline configuration used a base thickness of 56 μm , a background doping concentration of $6.0 \times 10^{16} \text{ cm}^{-3}$, front and rear surface recombination velocities of 1.0×10^5 and $1.0 \times 10^5 \text{ cm/s}$, respectively, and an operating temperature of 25 $^\circ\text{C}$.

Consistent with Section II-A, nine structural and electrical parameters were evaluated through joint-sensitivity screening. None of the candidate parameters was predetermined as an effective design variable. Pearson correlation coefficients were calculated between each candidate parameter and V_{oc} , J_{sc} , and FF , and the joint-sensitivity score S_p was obtained from the minimum absolute correlation across the three indicators. Parameters satisfying the application-specific criterion $S_p \geq 0.90$ were retained for the subsequent coarse-to-fine search.

As summarized in Table 1, base thickness, operating temperature, background doping concentration, front surface recombination velocity, and rear surface recombination velocity satisfied the joint-sensitivity criterion, with S_p values of 0.934, 0.934, 0.923, 0.903, 0.979, and 0.958, respectively. Substrate thickness, emitter distance, front texture angle, and base bulk recombination yielded S_p values of 0.729, 0.350, 0.665, and 0.839, respectively, and were not

retained. Substrate thickness was strongly correlated with V_{oc} and J_{sc} but showed a weaker association with FF , whereas front texture angle was strongly associated with J_{sc} and FF but only weakly associated with V_{oc} . These contrasting responses demonstrate the need for the joint criterion. The four unretained parameters were fixed at their baseline values. The five retained variables are hereafter denoted as base thickness t , operating temperature T , background doping concentration N_D , front surface recombination velocity S_f , and rear surface recombination velocity S_r . Their admissible ranges, sampling schemes, and coarse-grid level counts are summarized in Table 2. The exact sampled values used for the local refinement and one-dimensional sweeps are provided in Supplementary Table S2.

Table 1. Pearson correlation coefficients and joint-sensitivity screening results for the nine candidate device parameters

Parameters	Correlation Analysis				<i>Retained</i>
	V_{oc}	J_{sc}	FF	S_p	
Base Thickness	-0.996	0.934	-0.994	0.934	Yes
Temperature	-0.999	0.923	-0.999	0.923	Yes
Background Doping	0.967	-0.996	0.903	0.903	Yes
Front Surface Recombination	-0.994	-0.996	0.979	0.979	Yes
Rear Surface Recombination	-0.959	-0.982	-0.958	0.958	Yes
Substrate Thickness	-0.994	-0.998	-0.729	0.729	No
Emitter Distance	0.589	-0.350	0.604	0.350	No
Front Texture Angle	-0.665	0.991	-0.979	0.665	No
Base bulk recombination	0.865	0.839	0.875	0.839	No

* Parameters with $S_p \geq 0.90$ were selected as effective design variables. The sign of each Pearson coefficient indicates the direction of the relationship, whereas its absolute magnitude indicates the correlation strength.

Table 2. Effective design-variable ranges and PC1D coarse-grid sampling settings for the crystalline-silicon case study

Design Variables	Symbol	Admissible ranges	Sampling method/interval	Number of levels
Base Thickness	t (μm)	30.0 to 120.0	Linear (10.0)	10
Temperature	T (K)	285 to 330	Linear (5.0)	10
Background Doping Concentration	N_D (cm^{-3})	5.0E16 to 6.8E16	Linear (2.0E15)	10
Front Surface Recombination Velocity	S_f (cm/s)	500 to 1.0E5	Log spacing	10
Rear Surface Recombination Velocity	S_r (cm/s)	500 to 1.0E5	Log spacing	10

III-B. Step 2: Online coarse-to-fine optimization results

Step 2 was applied to the five design variables retained in Step 1 using the two-stage procedure described in Section II-B. The global coarse-grid search first identified the candidate optimal case, after which local high-resolution refinement identified the refined optimal case. One-dimensional sweeps were subsequently used to examine the local objective and constraint responses around the refined configuration.

III-B-1. Step 2-1: Global coarse-grid search and candidate optimal case identification

Using the five design variables retained in Step 1, a global coarse-grid exploration was performed across the predefined design space. The PC1D coarse grid comprised ten sampling levels for each variable, yielding $10^5=100,000$ full-factorial cases. Linear spacing was used for t , T , and N_D , whereas ten logarithmically spaced levels were used for S_f and S_r , consistent with the sampling settings in Table 2. During this exploration, each design case was evaluated sequentially in an online manner. For every case, the device model was generated, the performance indicators were extracted, and feasibility was immediately assessed based on the imposed V_{oc} , J_{sc} , and FF constraints. Feasible and infeasible cases were therefore classified and accumulated concurrently during the exploration.

To define an application-relevant feasible domain during online exploration, three minimum electrical-performance requirements were imposed on open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), and fill factor (FF). The threshold values were adopted as conservative, application-specific criteria informed by the reported performance of high-quality crystalline-silicon devices [13], [45].

First, a minimum threshold for open-circuit voltage was enforced to suppress excessive bulk and surface recombination and to preserve a sufficiently strong built-in electric field for effective charge carrier separation. Accordingly, the following constraint was applied:

$$V_{oc}^* \leq V_{oc} \quad (\text{V}) \quad (6)$$

where $V_{oc}^*=0.65 \text{ V}$ is the application-specific minimum open-circuit-voltage threshold adopted in this study.

Second, to ensure adequate optical absorption and photogenerated carrier collection under standard AM1.5G illumination, a lower bound was imposed on the short-circuit current density:

$$J_{sc}^* \leq J_{sc} \quad (\text{mA/cm}^2) \quad (7)$$

where $J_{sc}^*=32 \text{ mA/cm}^2$ is the application-specific minimum short-circuit-current-density threshold adopted in this study.

Third, a minimum fill factor requirement was introduced to prevent the optimization from favouring configurations with acceptable voltage or current but excessive resistive losses or degraded diode behavior:

$$FF^* \leq FF \quad (8)$$

where $FF^*=0.81$ is the application-specific minimum fill-factor threshold adopted in this study.

Together, these constraints define a physically meaningful and practically relevant feasible design space by imposing minimum acceptable electrical-performance requirements. Using short-circuit current density rather than total short-circuit current removes the direct dependence of the current-related feasibility criterion on device area, whereas V_{oc} and FF provide complementary intensive performance measures under the adopted one-dimensional device model.

For numerical implementation within the online optimization workflow, the inequality constraints were expressed as dimensionless normalized constraint functions, thereby enabling a uniform sign-based feasibility test for every simulated case during large-scale exploration.

Based on these definitions, the constrained optimization problem used in Step 2 was formulated as follows:

$$\begin{aligned}
&\text{Find} && \mathbf{x} = (t, T, N_D, S_f, S_r) \\
&\text{to maximize} && f(\mathbf{x}) = \eta \quad (\%) \\
&\text{subject to} && g_1(\mathbf{x}) = 1 - \frac{V_{oc}}{V_{oc}^*} \leq 0 \\
&&& g_2(\mathbf{x}) = 1 - \frac{J_{sc}}{J_{sc}^*} \leq 0 \\
&&& g_3(\mathbf{x}) = 1 - \frac{FF}{FF^*} \leq 0 \quad (9) \\
\\
&\text{where} && 30 \leq t \leq 120 \quad (\mu m) \\
&&& 285 \leq T \leq 330 \quad (K) \\
&&& 5.0 \times 10^{16} \leq N_D \leq 6.8 \times 10^{16} \quad (cm^{-3}) \\
&&& 500 \leq S_f \leq 1.0 \times 10^5 \quad (cm / s) \\
&&& 500 \leq S_r \leq 1.0 \times 10^5 \quad (cm / s)
\end{aligned}$$

where the design vector $\mathbf{x}$ represents the five effective design variables retained in Section III-A. The sign of each normalized constraint function was used to assign the feasibility status of every evaluated case.

Among the feasible cases, conversion efficiency was continuously compared during online exploration. Whenever a newly evaluated feasible design yielded a higher efficiency under the imposed constraints, the current best feasible configuration was updated in real time. After all 100,000 cases had been evaluated, Case 99100 was identified as the candidate optimal case without requiring a separate global post-processing stage. This configuration had $t = 30 \mu m$, $T = 285 K$, $N_D = 6.8 \times 10^{16} cm^{-3}$, $S_f = 500 cm/s$, and $S_r = 500 cm/s$, yielding $\eta = 17.5149\%$ under standard AM1.5G illumination. The complete set of design variables and corresponding performance metrics for this candidate optimal case is summarized in Table 3.

Table 3. Representative feasible configurations from the global PC1D coarse-grid search.

Case	Design Variables					Performances			Objective Function
	t [μm]	T [K]	N_D [cm^{-3}]	S_f [cm/s]	S_r [cm/s]	V_{oc} [V]	J_{sc} [mA/cm ²]	FF	η [%]
9490	120	285	6.0E16	900.82	500	0.650061	32.0012	0.817459	17.0054
9498	120	285	6.0E16	500	1622.97	0.650053	32.0041	0.817456	17.0067
9499	120	285	6.0E16	500	900.824	0.650075	32.0094	0.817456	17.0101
:	:	:	:	:	:	:	:	:	:
99098	30	285	6.8E16	500	1622.97	0.665628	32.0225	0.819538	17.4685
99099	30	285	6.8E16	500	900.824	0.666139	32.0508	0.819575	17.4982
99100*	30	285	6.8E16	500	500	0.66643	32.0667	0.819596	17.5149
99169	30	285	6.6E16	2924.02	900.824	0.665395	32.0001	0.819464	17.4486
99170	30	285	6.6E16	2924.02	500	0.66568	32.0156	0.819485	17.4650
:	:	:	:	:	:	:	:	:	:
99998	30	285	5.0E16	500	1622.97	0.660739	32.1383	0.818917	17.3898
99999	30	285	5.0E16	500	900.824	0.661172	32.1592	0.818955	17.4132
100000	30	285	5.0E16	500	500	0.661417	32.1709	0.818976	17.4265

* Candidate optimal case identified by the global PC1D coarse-grid search. Blue entries indicate configurations satisfying all imposed constraints.

III-B-2. Step 2-2: Local high-resolution refinement and one-dimensional sweep analysis

Starting from the candidate optimal case obtained in Step 2-1, a local high-resolution search was performed in its neighborhood to determine the refined optimal case within the feasible domain. This refinement stage used a finer discretization with smaller step sizes around the candidate solution, enabling detailed exploration of the local performance landscape under the same imposed constraints. Three levels were assigned to each of the five effective design variables, yielding $3^5=243$ full-factorial cases. The evaluated levels were $t = \{30, 33, 36\} \mu\text{m}$, $T = \{285, 286, 287\} \text{K}$, $N_D = \{6.70, 6.75, 6.80\} \times 10^{16} \text{cm}^{-3}$, and $S_f, S_r = \{500, 600, 700\} \text{cm/s}$.

During this high-resolution local re-sampling process, multiple design cases were automatically generated and evaluated using the same simulation engine, PC1D, employed in Steps 1 and 2. From these locally refined results, the refined optimal case was identified as the configuration that simultaneously satisfied all constraint conditions and yielded the maximum conversion efficiency within the refined feasible region.

Importantly, the local high-resolution refinement dataset and the one-dimensional sweep dataset served different purposes. The local refinement dataset, provided in Supplementary Table S3, was generated within a narrow neighborhood of the candidate optimal case using smaller step sizes and was used to identify the refined optimal case within the refined feasible region. In contrast, the automated one-dimensional sweeps shown in Fig. 3 were performed over broader variable-specific ranges to visualize the responses of conversion efficiency and the constraint metrics around the identified refined optimal case.

For each one-dimensional sweep, one effective design variable was varied over its prescribed sweep range, while the remaining variables were fixed at the refined optimal values. This procedure provided a visual and constraint-consistent interpretation of the selected refined optimum by showing how the objective function and imposed constraints varied as each design variable moved away from the selected configuration. Thus, Supplementary Table S3 provides the quantitative basis for refined optimal case identification, whereas Fig. 3 provides the corresponding sweep-based visualization and constraint-consistency interpretation.

The one-dimensional sweep results served two complementary purposes. First, local-response consistency was assessed by examining whether the conversion efficiency exhibited a smooth and physically plausible response around the refined optimum or feasible boundary,

depending on the design variable. This behavior reduced the likelihood that the selected solution was a grid-induced numerical artifact.

Second, constraint consistency was assessed by jointly examining the one-dimensional sweep profiles of conversion efficiency and the corresponding constraint metrics. These profiles showed that the selected refined optimal case remained within the feasible region while satisfying all imposed V_{oc} , J_{sc} , and FF constraints.

A representative example is shown in Fig. 3(c), which presents the one-dimensional sweep with respect to the background doping concentration. Within the admissible design-variable bounds specified in Table 2, the sweep showed that the highest feasible efficiency occurred at $N_D = 6.75 \times 10^{16} \text{ cm}^{-3}$, corresponding to Case H-91 in Supplementary Table S3. This configuration satisfied all imposed V_{oc} , J_{sc} , and FF constraints while yielding the highest conversion efficiency in the refined local dataset. Therefore, the selected refined optimal case was determined not by efficiency alone, but by simultaneous satisfaction of all performance constraints within the feasible region.

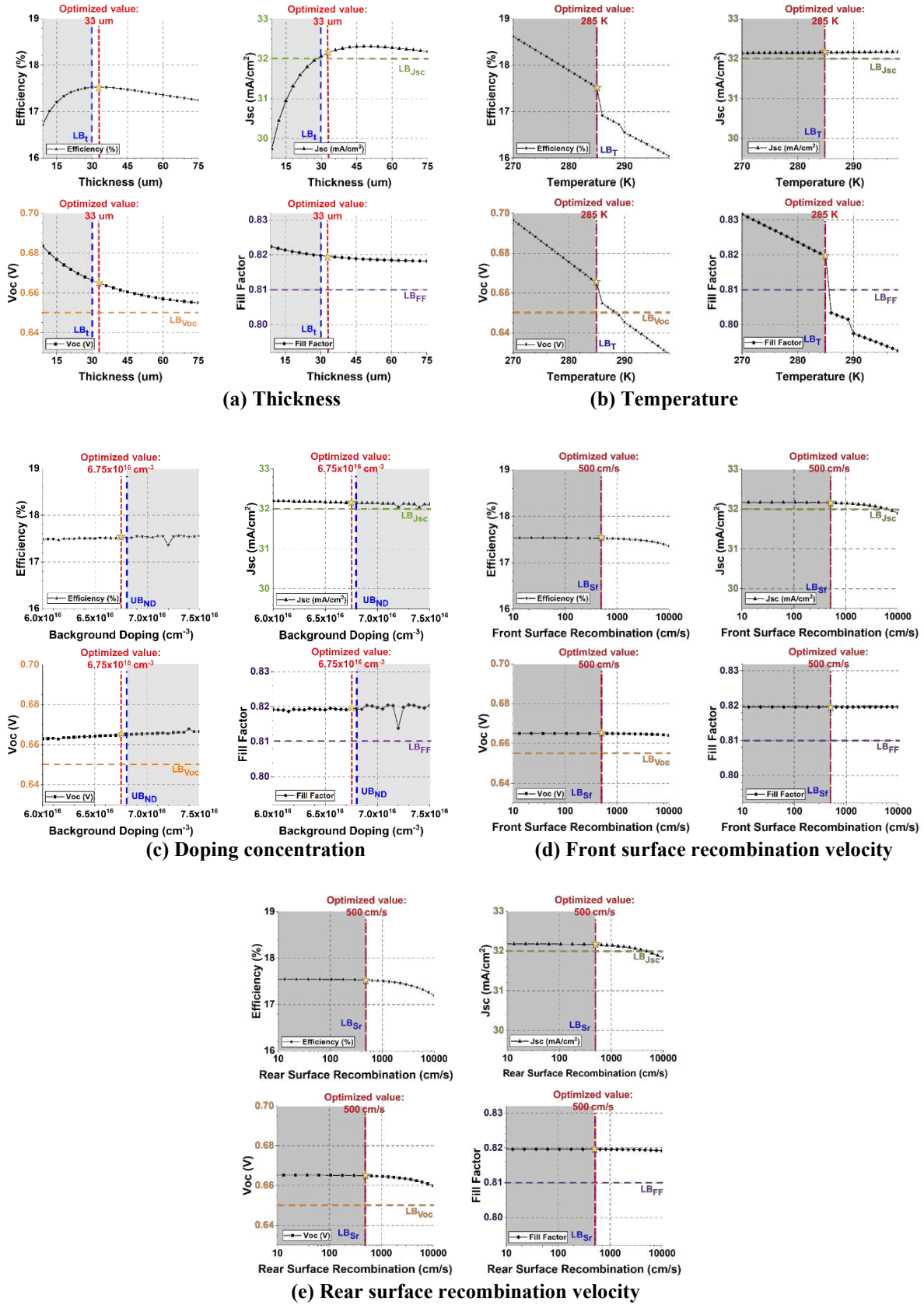


Figure 3. Automated one-dimensional sweep profiles over extended variable-specific ranges for visual interpretation of conversion efficiency and constraint metrics: (a) thickness, (b) temperature, (c) doping concentration, (d) front surface recombination velocity, and (e) rear surface recombination velocity

Through this integrated local high-resolution search and one-dimensional sweep-based intra-solver analysis, Step 2-2 provided numerical refinement of the candidate optimal case and constraint-consistent local interpretation of the resulting PC1D-derived refined optimal case. In the present application, the refined optimal case corresponded to Case H-91, characterized by $t = 33 \text{ } \mu\text{m}$, $T = 285 \text{ K}$, $N_D = 6.75 \times 10^{16} \text{ cm}^{-3}$, $S_f = 500 \text{ cm/s}$, and $S_r = 500 \text{ cm/s}$. This configuration yielded $\eta = 17.5249\%$ under standard AM1.5G illumination. Detailed design-variable and performance values are provided in Supplementary Table S3. In Step 3, the design-variable configuration of this PC1D-derived refined optimal case was compared with that of the independently obtained SCAPS refined optimum.

III-C. Step 3: Independent SCAPS-1D coarse-to-fine cross-solver assessment

In this subsection, Step 3 independently re-explored the design space using a reduced SCAPS-1D coarse grid and subsequently applied constraint-enforced local refinement around the resulting high-performance reference case. The same design-variable bounds, conversion-efficiency objective, and application-specific electrical constraints used in Step 2 were retained. Unlike the automated PC1D workflow, all SCAPS-1D cases were manually constructed and evaluated through the graphical user interface.

At the coarse level, the predefined design space was re-explored using SCAPS-1D at reduced resolution. The SCAPS coarse grid comprised four levels for t , four levels for T , three levels for N_D , and four logarithmically spaced levels for each of S_f and S_r , yielding $4 \times 4 \times 3 \times 4 \times 4 = 768$ full-factorial cases. Case V-33 yielded the highest conversion efficiency among the evaluated coarse SCAPS cases and was therefore selected as the high-performance reference case for local refinement. Because its J_{sc} value was slightly below the imposed threshold, V-33 was interpreted as a refinement-center case representing the SCAPS high-performance region rather than as the final feasible optimum.

At the refined level, three levels were assigned to each of the five design variables around V-33, yielding $3^5 = 243$ SCAPS-1D cases. The same objective function and constraint conditions were applied to all refined cases. Among the constraint-satisfying configurations, Case VH-91 yielded the highest conversion efficiency and was identified as the SCAPS-derived refined optimal case. VH-91 had $t = 33 \text{ } \mu\text{m}$, $T = 285 \text{ K}$, $N_D = 6.75 \times 10^{16} \text{ cm}^{-3}$, $S_f = 500 \text{ cm/s}$, and $S_r = 500 \text{ cm/s}$, which matched the design-variable configuration of the PC1D-derived refined optimal case H-91.

The primary cross-solver consistency criterion was the agreement of the independently derived refined optimal design-variable settings rather than strict numerical equality of the predicted performance metrics. Differences between PC1D and SCAPS-1D in numerical formulations, material databases, and boundary-condition treatments led to systematic discrepancies in V_{oc} , J_{sc} , FF , and conversion efficiency. Nevertheless, both independently executed coarse-to-fine searches converged to the same refined design-variable configuration. This agreement provided a direct cross-solver consistency check, reduced the likelihood that the refined optimum was a solver-specific numerical artifact, and supported the physical plausibility of the selected design. Table 4 summarizes the independent SCAPS coarse exploration and local refinement, while Table 5 directly compares the paired PC1D and SCAPS-1D results for representative refined configurations.

Table 4. Representative results from the independent SCAPS-1D coarse exploration and local refinement. Panel A presents coarse-level high-performance-region identification, and Panel B presents constraint-enforced local refinement around the SCAPS coarse reference case V-33.

Case	Design Variables					Performances			Objective Function
	t [μm]	T [K]	N_D [cm^{-3}]	S_f [cm/s]	S_r [cm/s]	V_{oc} [V]	J_{sc} [mA/cm^2]	FF	η [%]
A: Coarse exploration									
V-1	30	285	5.00E16	500	500	0.7060	32.1469	0.8211	18.6375
V-2	30	285	5.00E16	500	2924	0.7033	31.8084	0.8210	18.3670
V-3	30	285	5.00E16	500	17100	0.6943	30.4486	0.8206	17.3478
:	:	:	:	:	:	:	:	:	:
V-32	30	285	5.90E16	100000	100000	0.6767	27.9625	0.8190	15.4972
V-33*	30	285	6.80E16	500	500	0.7099	31.9576	0.8221	18.6519
V-34	30	285	6.80E16	500	2924	0.7071	31.5500	0.8219	18.3371
:	:	:	:	:	:	:	:	:	:
V-766	120	330	6.80E16	100000	2924	0.6046	32.0558	0.7808	15.1322
V-767	120	330	6.80E16	100000	17100	0.6041	31.8430	0.7809	15.0218
V-768	120	330	6.80E16	100000	100000	0.6036	31.6323	0.7810	14.9126
B: Local refinement									
VH-1	30	285	6.70E16	500	500	0.7098	31.9677	0.8220	18.6522
VH-2	30	285	6.70E16	500	600	0.7097	31.9677	0.8220	18.6513
VH-3	30	285	6.70E16	500	700	0.7097	31.9676	0.8220	18.6505
:	:	:	:	:	:	:	:	:	:
VH-82	33	285	6.70E16	500	500	0.7092	32.0058	0.8219	18.6544
VH-91**	33	285	6.75E16	500	500	0.7092	32.0007	0.8219	18.6545
VH-100	33	285	6.80E16	500	500	0.7093	31.9957	0.8219	18.6544
:	:	:	:	:	:	:	:	:	:
VH-241	36	287	6.80E16	700	500	0.7050	32.0078	0.8204	18.5131
VH-242	36	287	6.80E16	700	600	0.7050	32.0078	0.8204	18.5123
VH-243	36	287	6.80E16	700	700	0.7049	32.0077	0.8204	18.5115

* Highest-efficiency SCAPS coarse case used as the local-refinement center; ** best feasible SCAPS refined case. Blue entries indicate constraint-satisfying values; red entries indicate constraint-violating values. The SCAPS coarse grid comprises $4_t \times 4_T \times 3_{N_D} \times 4_{S_f} \times 4_{S_r} = 768$ cases, whereas the refined grid comprises $3^5=243$ cases.

Table 5. Direct PC1D–SCAPS-1D performance comparison for representative configurations in the refined search region, including the common refined optimum at Case C-91.

Case	Design Variables					V_{oc} [V]			J_{sc} [mA/cm ²]			FF			η [%]		
	t [μ m]	T [K]	N_D [cm ⁻³]	S_f [cm/s]	S_r [cm/s]	PM *	SV **	D_r ***	PM	SV	D_r	PM	SV	D_r	PM	SV	D_r
C-1	30	285	6.70E16	500	500	0.67	0.71	6.55	32.07	31.97	0.33	0.819	0.822	0.33	17.50	18.65	6.56
C-2	30	285	6.70E16	500	600	0.67	0.71	6.56	32.07	31.97	0.31	0.819	0.822	0.33	17.50	18.65	6.58
C-3	30	285	6.70E16	500	700	0.67	0.71	6.57	32.06	31.97	0.30	0.819	0.822	0.33	17.50	18.65	6.60
:	:	:	:	:	:	:	:	:	:	:	:	:	:	:	:	:	:
C-90	33	285	6.70E16	700	700	0.66	0.71	6.67	32.14	31.97	0.54	0.819	0.822	0.34	17.50	18.63	6.45
C-91 ****	33	285	6.75E16	500	500	0.66	0.71	6.67	32.16	32.00	0.48	0.820	0.822	0.28	17.52	18.65	6.45
C-92	33	285	6.75E16	500	600	0.66	0.71	6.67	32.15	32.00	0.47	0.820	0.822	0.28	17.52	18.65	6.46
:	:	:	:	:	:	:	:	:	:	:	:	:	:	:	:	:	:
C-241	36	287	6.80E16	700	500	0.66	0.70	6.91	32.21	32.01	0.63	0.818	0.820	0.36	17.36	18.51	6.62
C-242	36	287	6.80E16	700	600	0.66	0.70	6.91	32.21	32.01	0.62	0.817	0.820	0.36	17.36	18.51	6.64
C-243	36	287	6.80E16	700	700	0.66	0.70	6.92	32.20	32.01	0.60	0.817	0.820	0.36	17.36	18.51	6.65

*PM: proposed method results; **SV: SCAPS-1D results; *** D_r : relative percentage difference calculated as $D_r = |SV - PM| / PM \times 100\%$; ****: refined optimal case. The prefix “C” denotes paired configurations used for PC1D–SCAPS-1D comparison. Relative percentage differences were calculated from the unrounded simulation values; displayed performance values were rounded independently.

As shown in Table 5, PC1D and SCAPS-1D produced closely comparable J_{sc} and FF values across the representative refined configurations, with relative differences of 0.30–0.63% and 0.28–0.36%, respectively. Larger but consistently directed differences were observed for V_{oc} and conversion efficiency, with relative differences of 6.55–6.92% and 6.45–6.65%, respectively, and SCAPS-1D predicting higher values. Importantly, both simulators identified the same refined design-variable configuration at Case C-91. The narrow and systematic ranges of the observed differences suggest solver-dependent offsets in absolute performance prediction rather than irregular case-specific divergence. Accordingly, the common refined configuration provides numerical evidence of cross-solver consistency, although it does not imply equality of the predicted performance metrics or experimental validation.

III-D. Computational cost and practical executability

This subsection evaluates the computational cost and practical executability of the proposed workflow. The analysis considers the measured cost of the implemented PC1D and SCAPS-1D searches and the estimated computational burden of two hypothetical full-domain fine-grid scenarios.

A total of 100,243 device configurations were evaluated using the automated PC1D–in-house environment during Step 2, comprising 100,000 coarse-grid cases and 243 local-refinement cases. Each case required an average computation time of approximately 1.1 s, resulting in a total execution time of approximately 110,267 s. The physical device model was not simplified; instead, device construction, performance evaluation, feasibility screening, and current-best tracking were integrated into a single simulation loop. This online structure removed a separate post-processing pass for feasibility screening and optimum selection but did not reduce the number of prescribed PC1D simulations.

The SCAPS-based procedure in Step 3 performed an independent reduced-resolution coarse exploration using 768 cases, followed by a 243-case constraint-enforced local refinement. At

the coarse level, the predefined design space was re-explored at reduced resolution to identify the SCAPS high-performance reference case used as the center of local refinement. At the refined level, 243 cases were evaluated around this SCAPS-derived coarse reference using smaller step sizes, and the best feasible configuration was identified as the SCAPS refined optimum. In total, 1,011 SCAPS-1D cases were manually constructed and evaluated. With an average computation time of approximately 60 s per case, the total computation time was 60,660 s, as summarized in Supplementary Table S4. Although this manual procedure was substantially more expensive per case than the automated PC1D workflow, the reduced coarse grid and focused local refinement avoided a full high-resolution exploration of the entire design space.

For reference, a full-domain extrapolation of the adopted variable-specific fine-sampling definitions was considered. As detailed in Supplementary Table S5, this extrapolation required 31, 46, 37, 32, and 32 sampling levels for t , T , N_D , S_f , and S_r , respectively. The resulting full-factorial case count was

$$N_{fine}^{global} = 31 \times 46 \times 37 \times 32 \times 32 = 54,028,288, \quad (10)$$

At the measured average PC1D execution time of approximately 1.1 s per case, serial execution would require approximately 59.4×10^6 s, corresponding to about 687.9 days. This estimate illustrates the computational burden of applying fine sampling over the entire multivariable design domain and explains why high-resolution exploration is restricted to a local region in the proposed workflow.

Accordingly, an illustrative full-domain fine-grid scenario was considered to provide a computationally tractable comparison. Each of the five variables was assigned 20 sampling levels over its complete admissible range, corresponding to twice the number of levels used per variable in the global coarse-grid search. Linear spacing was applied to t , T , and N_D , whereas logarithmic spacing was retained for S_f and S_r . This scenario yielded

$$N_{20}^{global} = \prod_{j=1}^5 n_j = 20^5 = 3,200,000, \quad (11)$$

where $n_j = 20$ for each design variable. Using the measured average PC1D execution time of approximately 1.1 s per case, this scenario would yield 3,200,000 configurations and an estimated serial computation time of 3.52×10^6 s, or approximately 40.7 days. The 20-level scenario was not intended to reproduce the exact variable-specific increments of the local refinement; rather, it provided an illustrative benchmark for the combinatorial computational growth associated with increasing sampling density over the full design domain. This hypothetical search was not executed, and the wall-clock estimate assumed sequential execution without parallel processing.

For direct comparison, the four computational scenarios were as follows:

- (i) the implemented PC1D coarse-to-fine search evaluated 100,243 cases in 110,267 s, or approximately 30.6 h;
- (ii) the SCAPS-1D assessment evaluated 1,011 cases in 60,660 s, or approximately 16.9 h;
- (iii) the illustrative 20-level full-domain grid would require 3,200,000 cases and 3.52×10^6 s, or approximately 40.7 days; and
- (iv) the full-domain variable-specific fine-sampling extrapolation would require 54,028,288 cases and 5.94×10^7 s, or approximately 687.9 days.

Relative to the implemented PC1D search, the two hypothetical full-domain scenarios correspond to approximately 32-fold and 539-fold increases in both case count and serial

computation time, respectively. These comparisons show that the coarse-to-fine workflow evaluates the complete prescribed coarse grid while restricting fine sampling to a local high-performance region, thereby avoiding the combinatorial computational burden of full-domain fine-grid exploration. Detailed measured and estimated computation times are provided in Supplementary Table S4.

IV. Discussion

This section discusses the advantages and limitations of the proposed constraint-aware online optimization workflow. The discussion focuses on the structural benefits of online constraint-integrated exploration, the cross-solver numerical consistency of the selected design, and the practical trade-offs associated with the adopted sampling strategy.

IV-A. Advantages of the proposed workflow

A primary advantage of the proposed workflow is the integration of feasibility assessment and objective-based ranking within a single online simulation loop. Conventional workflows generally generate a complete dataset before performing feasibility filtering and optimal-case selection as separate post-processing steps. In contrast, the proposed workflow evaluates the constraints, classifies feasible and infeasible cases, and updates the current best feasible configuration during case generation. Although all prescribed cases are still evaluated, this integration makes feasibility information and current-best tracking immediately available and removes a separate global filtering and ranking pass. It therefore reduces workflow fragmentation without implying early stopping or a reduction in the number of simulations.

The coarse-to-fine search strategy further improves the computational practicality and interpretability of the workflow. The global coarse-grid search systematically covers the prescribed design domain and identifies a candidate optimal case, whereas local high-resolution refinement concentrates finer sampling around the resulting high-performance region. The automated one-dimensional sweep analysis then reveals how conversion efficiency and the constraint metrics vary around the refined optimal configuration. The computational comparison further showed that the two hypothetical full-domain scenarios would require approximately 32-fold and 539-fold more cases than the implemented PC1D search. Thus, the workflow not only identifies a refined optimum but also reveals local response trends, feasible boundaries, and parameter–performance trade-offs while avoiding the combinatorial burden of full-domain fine-grid exploration.

The cross-solver analysis provides an additional advantage by assessing numerical consistency across independent simulation environments. The independently executed SCAPS-1D coarse exploration identified a corresponding high-performance design region, and its subsequent local refinement converged to the same design-variable configuration as the PC1D-derived refined optimum. This agreement does not constitute experimental validation; rather, it reduces the likelihood that the refined configuration is a solver-specific numerical artifact and supports the physical plausibility of the selected design. The consistent design selection, despite systematic differences in the predicted absolute performance values, supports the practical use of the workflow for pre-fabrication photovoltaic-device exploration.

IV-B. Limitations and practical trade-offs

The computational advantage of the coarse-to-fine strategy is accompanied by a scalability trade-off associated with uniform grid sampling in the global-search stage. The coarse grid systematically covers the prescribed design space and can identify high-performance regions without prior knowledge of their locations. Combined with local high-resolution refinement, this structure substantially reduces the computational burden relative to applying fine sampling over the full design domain. However, the global stage does not adaptively prioritize promising regions during early exploration, and the number of full-factorial cases increases

multiplicatively with the number of variables and sampling levels. The principal limitation therefore concerns scalability relative to adaptive search strategies, rather than the ability of the workflow to identify promising designs within the evaluated five-variable design space.

A second limitation concerns the scope of the cross-solver assessment. The refined configuration was evaluated through PC1D-based local refinement, one-dimensional response analysis, and an independent SCAPS-1D coarse-to-fine assessment. Agreement between the two simulators in the selected refined design-variable configuration reduces the likelihood of a solver-specific numerical artifact and supports the physical plausibility of the result. Nevertheless, the device was not fabricated or experimentally measured. The cross-solver agreement should therefore be interpreted as numerical consistency rather than experimental validation.

The present study is also limited to cell-level computational design. Module-scale energy-yield analysis, techno-economic assessment, and life-cycle evaluation were outside the scope of this work, and the reported results should not be interpreted as direct system-level performance or cost predictions. The intended role of the workflow is to narrow the feasible design space, identify constraint-satisfying high-performance regions, and provide interpretable pre-fabrication guidance before experimental or system-level evaluation.

Future work could incorporate adaptive or learning-based sampling to improve search efficiency in higher-dimensional design spaces. Such strategies could direct simulations toward promising regions using information acquired during early exploration, although their added algorithmic complexity should be balanced against the transparent feasible-domain mapping and reproducible coverage afforded by uniform sampling. Experimental fabrication and module- or system-level assessments will also be required to determine whether the numerically identified design advantages persist beyond the cell-level simulation environment. A complementary direction is to extend the workflow to advanced crystalline-silicon architectures, including passivated emitter and rear cell (PERC), tunnel oxide passivated contact (TOPCon), and silicon heterojunction devices. Such extensions would require architecture-specific physical models, design variables, feasibility criteria, and independent numerical and experimental assessment procedures.

V. Conclusion

This study developed a constraint-aware online coarse-to-fine optimization workflow for crystalline-silicon photovoltaic device design. By integrating automated model generation, performance extraction, feasibility classification, and current-best tracking into a single simulation loop, the workflow converts conventional post-processing-based design exploration into an active optimization process. The workflow was demonstrated using a multilayer crystalline-silicon solar cell. Joint-sensitivity-guided variable selection defined a compact and physically meaningful design space, and the online coarse-to-fine strategy identified a refined optimal case under explicit electrical constraints. Local high-resolution refinement and automated one-dimensional sweeps characterized the objective and constraint behavior around the refined optimum. An independently executed SCAPS-1D coarse-to-fine search converged to the same refined design-variable configuration as the PC1D-based workflow, providing a cross-solver consistency check and reducing the likelihood of a solver-specific numerical artifact. The computational analysis showed that the workflow removes a separate post-processing pass and avoids full-domain high-resolution refinement through a reduced SCAPS coarse grid and focused local refinement. Beyond reporting a single optimum, the workflow provides design guidance by revealing feasible regions, constraint boundaries, and performance trade-offs. Therefore, the proposed workflow provides a practical and physically interpretable computational foundation for pre-fabrication photovoltaic energy-conversion device optimization, particularly for design problems requiring transparent feasibility assessment, efficient exploration, and cross-solver consistency assessment.

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Author contributions

Aliaa Nabila Abdul Mutaali: Software, Investigation, Formal analysis, Data curation, Validation, Visualization, Writing – original draft.

Joungha Lee: Conceptualization, Methodology, Validation, Supervision, Writing – original draft, Writing – review & editing.

Seung Beop Lee: Conceptualization, Methodology, Supervision, Project administration, Resources, Writing – review & editing.

All authors reviewed and approved the final manuscript.

Competing interests

The authors declare no competing interests.

Data availability

The datasets generated and analyzed during the current study are provided in Supplementary Data S1. Additional supporting data are available from the corresponding author upon reasonable request.

Code availability

The complete in-house automation scripts are not publicly deposited because they contain laboratory-specific implementation and file-management components. The algorithmic workflow, case-representation scheme, decision rules, parameter settings, and pseudocode required to understand and independently reimplement the proposed method are provided in the manuscript and Supplementary Information. The code version used to generate the reported results will be made available to editors and reviewers upon request. Non-proprietary components are available from the corresponding author for non-commercial research purposes upon reasonable request.

Declaration of generative AI and AI-assisted technologies

During the preparation of this manuscript, the authors used ChatGPT (OpenAI) for limited assistance with English-language editing, structural consistency, and presentation. The tool was not used to generate research data, perform simulations, analyse the results, or determine the scientific conclusions. All AI-assisted text was critically reviewed and revised by the authors, who take full responsibility for the content of the manuscript.

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Figure Legends

Figure 1. Overview of the proposed constraint-aware online coarse-to-fine optimization approach. Step 1 performs automated virtual-device construction and joint-sensitivity-guided selection of effective design variables. Step 2 evaluates each simulated case online, classifies feasible and infeasible cases, updates the current best feasible design, and identifies candidate and refined optimal configurations through PC1D-based coarse-to-fine exploration and one-dimensional sweep analysis. Step 3 independently performs a reduced-grid SCAPS-1D coarse exploration followed by constraint-enforced local refinement to assess cross-solver numerical consistency.

Figure 2. Schematic multilayer crystalline-silicon device structure used in the case study and the five variables retained by joint-sensitivity screening

Figure 3. Automated one-dimensional sweep profiles over extended variable-specific ranges for visual interpretation of conversion efficiency and constraint metrics: (a) thickness, (b)

temperature, (c) doping concentration, (d) front surface recombination velocity, and (e) rear surface recombination velocity

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