Reflow profiling with the aid of machine learning models

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Abstract

Purpose – This paper aims to propose a method to quickly set the heating zone temperatures and conveyor speed of the reflow oven. This novel approach intensely eases the trial and error in reflow profiling and is especially helpful when reflowing thick printed circuit boards (PCBs) with bulky components. Machine learning (ML) models can reduce the time required for profiling from at least half a day of trial and error to just 1 h.

Design/methodology/approach – A highly compact computational fluid dynamics (CFD) model was used to simulate the reflow process, exhibiting an error rate of less than 1.5%. Validated models were used to generate data for training regression models. By leveraging a set of experiment results, the unknown input factors (i.e. the heat capacities of the bulkiest component and PCB) can be determined inversely. The trained Gaussian process regression models are then used to perform virtual reflow optimization while allowing a 4°C tolerance for peak temperatures. Upon ensuring that the profiles are inside the safe zone, the corresponding reflow recipes can be implemented to set up the reflow oven.

Findings – ML algorithms can be used to interpolate sparse data and provide speedy responses to simulate the reflow profile. This proposed approach can effectively address optimization problems involving multiple factors.

Practical implications – The methodology used in this study can considerably reduce labor costs and time consumption associated with reflow profiling, which presently relies heavily on individual experience and skill. With the user interface and regression models used in this approach, reflow profiles can be swiftly simulated, facilitating iterative experiments and numerical modeling with great effectiveness. Smart reflow profiling has the potential to enhance quality control and increase throughput.

Originality/value – In this study, the employment of the ultimate compact CFD model eliminates the constraint of components' configuration, as effective heat capacities are able to determine the temperature profiles of the component and PCB. The temperature profiles generated by the regression models are time-sequenced and in the same format as the CFD results. This approach considerably reduces the cost associated with training data, which is often a major challenge in the development of ML models.

Keywords Gaussian process regression (GPR), Computational fluid dynamics (CFD), Reflow soldering

Paper type Research paper

1. Introduction

Reflow soldering is a technique that temporarily applies solder paste to contact pads of numerous surface mount components. Following that, the entire assembly is heated under controlled temperatures, causing the solder paste to melt and form robust interconnections (Lau *et al.*, 2016). In the reflow process, a temperature curve over time is known as a reflow profile. Reflow profiling is an optimization process to determine the heating duration and temperatures of several critical points on the board (Lee, 1999). Because of the uneven distribution of components' heat capacities, it is impractical to reach a uniform temperature across the board. For bulky components, the temperatures of the solder joints must reach the minimum requirement, which ensures proper wetting and intermetallic compound formation (Salam *et al.*, 2004). Meanwhile, the temperature must be regulated to avoid damaging small-sized components due to excessive heating or thermal shock (Ha *et al.*, 2022). The acceptable temperature range during the reflow process is known as the process window. The aim is to ensure that all profiles are well inside the process window by effectively controlling the two extremums. As depicted in Figure 1, the upper limit is the board surface temperature, whereas the lower limit is the temperature of the solder joint under the bulkiest component. To create a robust bond through the formation of tin–copper intermetallics, the solder supplier specifies that the peak temperature should fall within the range of 230–260°C and the time above liquidus (TAL) should be between 30 and 100 s (Indium Corporation, 2023). Additionally, the ramp profile is required to be within 0.5–2.5°C/s. Reflow recipe, namely, conveyor speed and oven temperatures, are the key factors primarily determining the shapes of the reflow profiles. When using a convection oven with over ten heating zones, the factor count of the reflow recipe can reach two digits, making it more intricate.

To date, profiling relies heavily on individual experience and skill (Gao *et al.*, 2005). The method introduced in this study uses machine learning (ML) models to improve the accuracy and efficiency of the reflow process. This approach can significantly reduce the complexity of the iterative profiling work and has the potential to enhance throughput.

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Figure 1 Two extremums of the reflow profile

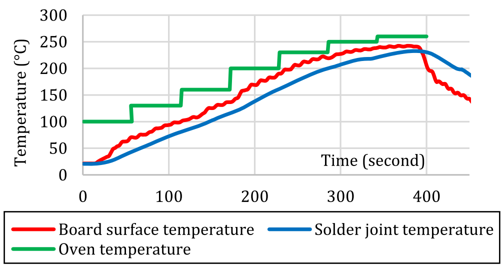

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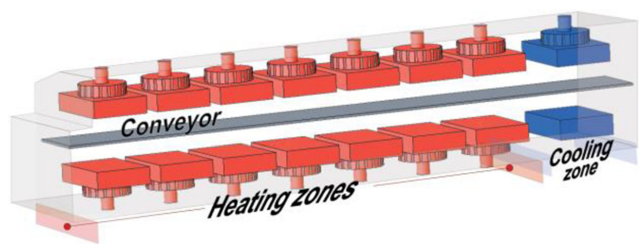
Figure 2 Configuration of the seven-zone oven



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Lots of efforts have been made to study the reflow soldering process using analytical or numerical methods. Gao provided a convenient method to develop reflow recipes for a specific reflow profile (Gao *et al.*, 2008). Mannan studied the behavior of solder paste using computational fluid dynamics (CFD) modeling (Mannan *et al.*, 2000). Abdul Aziz presents an effective numerical method to study pin shape during wave soldering (Abdul Aziz *et al.*, 2014). Lai studied the influence of uneven thermal mass distribution during reflow (Lai *et al.*, 2021, 2022a). Whalley presented a very simple approach to model the reflow process and got an extremely accurate prediction (Whalley, 2004).

In this work, the temperature change of printed circuit board (PCB) assembly was simulated using CFD modeling. To validate the CFD models, field measurements with three profiling boards were carried out. Identifying the reflow recipes for each assembly is a typical inverse problem, which necessitates trial and error. To ease the computation cost, the ML technique is used to address this inverse problem.

There are several prior research that has used ML techniques in the reflow process. Parviziomran used data-driven models to study self-alignment during reflow (Parviziomran *et al.*, 2019). Lai used deep learning models to generate the temperature contours during reflow (Lai *et al.*, 2022d). Jing used a genetic algorithm to predict the temperature curves of PCB assemblies (Jing *et al.*, 2021). Lai used ML models to specify reflow recipes for PCB with lidded ball grid array (BGA) packages (Lai *et al.*, 2023, 2022c).

The use of ML models in this study enables the rapid generation of temperature profiles in the same format as the measurement data, representing a significant improvement over the authors' previous approaches where only peak temperature and TAL were available as outputs (Lai *et al.*, 2023, 2022b). The algorithms play the roles of heat transfer of the forced convection and transient conduction, which are the two dominant heat transfer mechanisms of the reflow soldering process. Given the current high computing power available, ML models can reduce the time required for profiling from at least half a day of trial and error to just one hour.

2. Field measurement and computational fluid dynamics modeling

2.1 Field measurement

The study used a convection oven with seven heating zones, as illustrated in Figure 2. The temperature of each heating zone can be regulated independently, which determines the shapes of the reflow profile. The conveyor speed is another key factor of the reflow recipe, which determines the heating duration. The zone temperatures and conveyor speeds were set according to Table 1. Four conveyor speeds were examined separately to allow for the model's independence regarding heating duration.

As shown in Figure 3, there were three samples, which are lidded, lidless and ceramic packages, respectively. Three components are used to ensure that the proposed methodology can handle packages with various packaging designs and materials. Thermocouples were attached to the top of PCBs to monitor the board surface temperature. On the undersides of the boards, thermocouples were attached to the copper pads under the BGA to monitor the solder joints' temperatures, as shown in Figure 4. At the melting point, the solder material absorbs and dissipates latent heat, creating a plateau on the temperature plot, which is evidence that the solder temperature was successfully captured (Dušek *et al.*, 2016). A traveling thermal profiler was used to collect data within the oven with a precision of ± 1°C.

2.2 Computational fluid dynamics modeling

The ultimate compact CFD model built in ANSYS-FLUENT is shown in Figure 5. Three samples share the same structure but with different dimensions, as shown in Table 2. The component was entirely integrated into a single piece, and so has PCB. Because of the trend of heterogeneous integration technology, advanced package features varied designs such as redistribution layers, interposers and multiple chiplets (Pan *et al.*, 2022). It is not feasible to use detailed models because of their variety and complexity (Lai *et al.*, 2022b). Instead, ultimate compact modeling was used to make the model universal, which means package-structure independence. This is the biggest challenge in striking a balance between accuracy and application requirements.

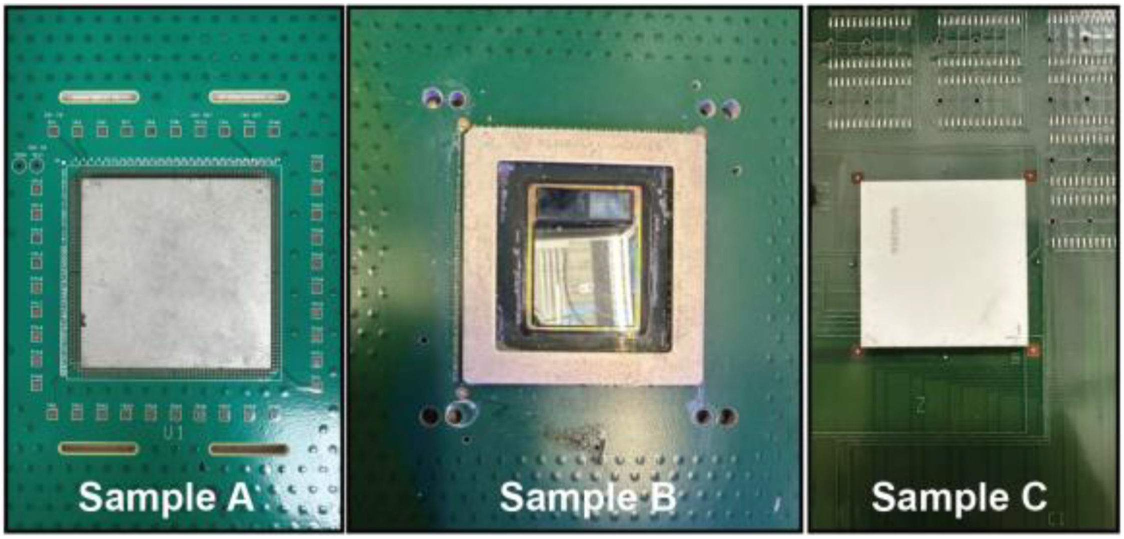
The quarter-symmetric model was divided into a number of control volumes using polyhedral meshing. The SIMPLE algorithm was used to enforce mass conservation and to obtain the pressure field. k-ε model was selected for the turbulent flow calculations. Mesh sensitivity studies were carried out for a

Table 1 Zone temperatures and conveyor speeds

Zone temperature (°C)							Conveyor speed
1	2	3	4	5	6	7	(cm/min)
100	130	160	160	170	225	265	45/ 40/ 35/ 30

Source: Authors' own work

Figure 3 Three samples for field experiment



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steady-state simulation. A smaller control volume was applied until monitor points for solder temperatures reached a steady solution, and the residual error values have reduced to 10^{-3} below. The body size of the component and PCB was finalized at 1 mm, and the maximum size of the air was set at 5 mm.

Latent heat must be taken into account since solder undergoes phase change during reflow. The solder material used is SAC305, which undergoes phase change at 217°C. The densities of the component and PCB were set as 2,300 kg/m^3 and 2,100 kg/m^3, respectively. It is important to note that the densities and thermal properties do not hold any reference significance. The modeling was designed to fine-tune using the specific heat of the component and PCB to establish the correlation with measurement results. The temperature change of the PCB assembly is determined by the effective heat capacity and oven temperatures.

To account for the velocity fields above and below the PCB, it is necessary to individually specify the flow rate of inlets. The temperature change of two pieces of aluminum boards was used to set the boundary condition of the CFD model. To ensure unidirectional heat transfer, fiberglass was used to interrupt the thermal conduction between two boards, as shown in Figure 6. Figure 7 demonstrates that the energy output from the upper outlet exceeds that of the lower outlet.

2.3 Model validation

The temperature profiles of the board surface and the solder joint were monitored for model validation. The measurement results at four different conveyor speeds, as presented in Figure 8, were compared to the CFD model to establish a correlation. The peak temperature and TAL of the simulation results were used to compare to those of the measurement results. The CFD model demonstrated an error rate of below 1.5%, indicating that the ultimate compact model is capable of effectively simulating the reflow process.

Figure 4 Attachment of thermocouple

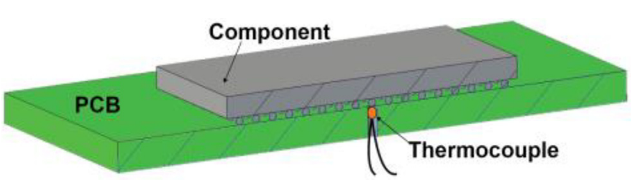

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Figure 5 The compact CFD model

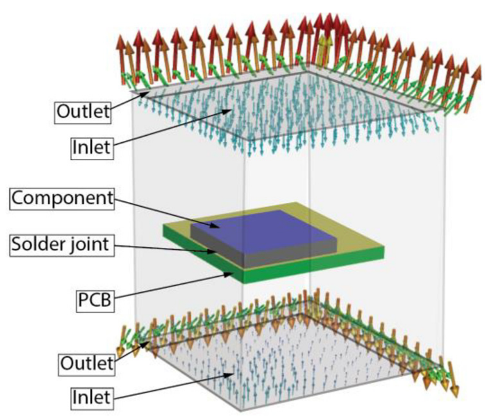

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Table 2 Dimensions of three samples

Part	Sample A (mm)	Sample B (mm)	Sample C (mm)
PCB	140 × 90 × 3	300 × 380 × 5	230 × 250 × 1.9
Component	47.5 × 47.5 × 3.33	61 × 61 × 4.3	32.5 × 32.5 × 3
Solder	Height: 0.45 Diameter: 0.6 Pitch: 1.0	Height: 0.4 Diameter: 0.75 Pitch: 0.8	Height: 0.5 Diameter: 0.6 Pitch: 1.0

Source: Authors' own work

Figure 6 Temperature measurement for aluminum boards

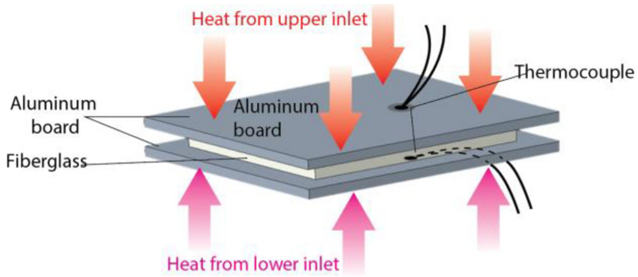

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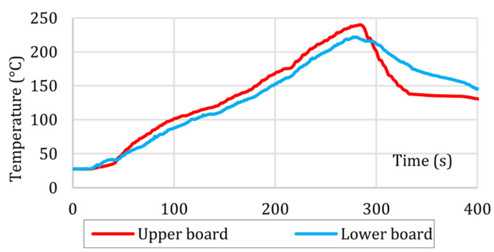
Figure 7 Temperature profiles of aluminum boards



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3. Machine learning modeling

The ML models used in this study provide interpolation for the restricted training data and quicker response times than those achieved through CFD modeling. To provide physical support for the ML model, the training data were automatically generated by the programmed CFD models.

3.1 Model training

As shown in Figure 9, ML models predict the temperature profiles in a time sequence, which aligns with the CFD results. The output temperatures of one step are used as inputs for the next step. The data demand is low because a one-time simulation of the reflow process can generate hundreds of data (one set of data per second). To address the varied convective flow during the heating and cooling, two ML models were needed for both PCB and solder joints.

Five CFD models with different levels in each geometry factor are shown in Table 3. These models were used to produce data via three reflow recipes, which can be found in Table 4. The effective heat capacities of both the component and PCB were intentionally designed to five different levels. The CFD models produced 375 sets of results altogether, which were used to train the ML models.

Figure 8 Reflow profiles at three conveyor speeds

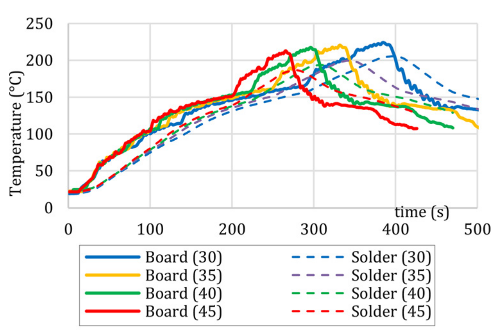

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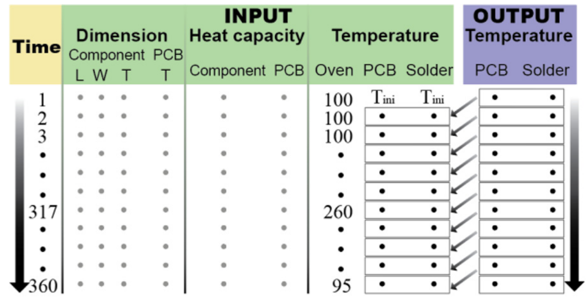
Figure 9 Input and output factors of the ML model



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3.2 The performance of machine learning models

Regression learner in MATLAB provides a range of algorithms to train and validate regression models. Once multiple models have been trained, the optimal model can be selected by assessing their validation errors in parallel. Four Gaussian process regression models were selected. The root mean square error (RMSE) of each model is below 0.1 with fivefold cross-validation. Given that the data source is a physical model devoid of interfering noise, achieving high accuracy in predictions is not surprising and means regression models are well-suited to replace CFD modeling.

4. Application of the reflow recipe generator

4.1 Workflow of the recipe generator

Figure 10 shows the workflow chart for performing reflow profiling using the reflow recipe generator for new assemblies.

Table 3 Levels of geometry factors

CFD model	Component thickness (mm)	Component length (mm)	Component width (mm)	PCB thickness (mm)
1	3.33	47.5	47.5	3.0
2	4.3	61.0	61.0	5.0
3	3.0	32.5	32.5	1.9
4	2.2	24.0	24.0	1.4
5	1.8	12.0	12.0	1.0

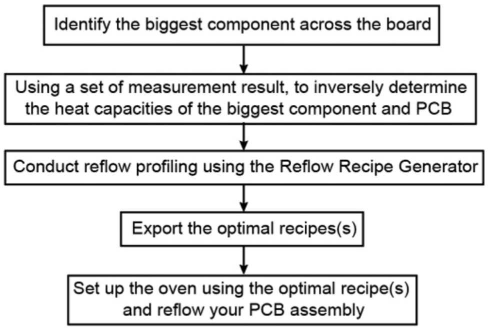
Source: Authors' own work

Table 4 Levels of reflow recipes

Zone temperature (°C)							Speed
1	2	3	4	5	6	7	(cm/min)
100	110	130	140	170	200	230	25
100	135	160	190	220	260	280	25
100	130	160	195	230	260	275	45

Source: Authors' own work

Figure 10 Workflow of the reflow profiling



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The first step involves identifying the largest component and attaching thermocouples to the central solder ball, as demonstrated in Figure 4. These thermocouples are used to monitor the temperatures of the coldest joints across the board, whereas other thermocouples are attached to the PCB surface to monitor the hottest temperatures. The subsequent step entails configuring the oven using the default recipe from Table 1, with the conveyor speed set at 35 cm/min, and collecting data via the thermocouples. The recipe generator can then use the golden section searching approach to inversely determine the heat capacities of the component and PCB, which are the two unknown variables. Following this, the reflow profiling work can be carried out virtually through the user interface. Once the two extreme limit profiles are centered within the safe band, the corresponding recipes can be deemed optimal.

4.2 Golden section searching

The golden-section search is a technique for searching an extremum of a function inside a preset range. For a unimodal function, the extremum can be found by iteratively narrowing the range of values on the specified interval. The interval width used in each iteration is based on the golden ratio (i.e. 0.618), which offers maximal efficiency (Bo *et al.*, 2009). The peak temperature measured with the initial recipe is used to inversely seek the heat capacities of the package and PCB. By applying equation (1), the inverse problem of seeking the heat capacities is transferred into a unimodal function:

$$f(c_p) = abs(T_{prediction} - T_{measurement}) \tag{1}$$

c_p = heat transfer of Package or PCB (J/kg K);
$T_{prediction}$ = peak temperature of prediction (°C); and
$T_{measurement}$ = peak temperature of measurement (°C).

Initially, the heat capacity of the PCB is calculated as its temperature remains unaffected by the other components. Subsequently, the heat capacity of the component can be calculated. The maximum error allowed is 30, implying that the iteration will cease once the difference of the target function is below 30. Typically, after 5 or 6 iterations, two heat capacities can be acquired.

4.3 Safe band

During the optimization process, the safe band indicates the process window within which the reflow profiles should be centered (Norman R. Cox, 1992). Two profile shapes are taken into consideration: ramp/soak/spike and ramp-to-peak profiles. The boundaries of the safe band are established using the solder paste material's spec sheet, as shown in Table 5. The safe band allows the predicted profiles to be visually examined to determine whether they meet the qualifying criteria.

4.4 Tips for reflow profiling

The primary aim of reflow profiling is to align the reflow profiles within the safe band. When the profiles are located too close to the safe band's boundary, a small manufacturing variation may cause the profiles to move out of the process window. In such instances, reducing the conveyor speed is a viable quality control solution. Along with peak temperatures and TAL, the gap between two peak temperatures denotes the thermal differential across the board. If the peak temperature gap is too big, using the ramp/soak/spike profile is recommended to decrease the difference. Soaking enables the PCB assembly to attain a relative equilibrium across the board before solder melting occurs.

In reflow profiling, peak temperature should receive greater attention than TAL due to measurement tolerance. Thermocouples used to measure solder temperature are connected to pads rather than directly to solder joints, and the solder temperature persists around 210°C for some time due to latent heat. As a result, measurement error can be magnified into a significant time-based error. Fortunately, TAL is typically provided with a large process window ranging from 30 to 120 s.

4.5 Prediction results

Using the optimal recipe, the ramp/soak/spike profile for Sample 1 was collected and compared with the predicted model profile shown in Figure 11. The recipe generator performed well, with the small flaw of the solder's peak temperature being 3°C higher than the measurement results. The ramp-to-peak profile for sample 2 is illustrated in Figure 12, with both the PCB and solder's peak temperatures being 3–4°C higher than the predicted values. Figure 13 displays the ramp/soak/spike profile for Sample 2 at a slow speed of 25 cm/min. The reflow recipe generator performed well overall, with both extreme limit profiles being safely within the safe band.

5. Conclusion

The utilization of a highly compact CFD model in this study eliminates the limitation imposed by the variation of the

Table 5 Parameter recommendation for SAC305

Reflow profile parameter	Acceptable
Ramp profile rate (average ambient to peak)	0.5–2.5°C/s
Soak zone duration	30–120 s
Soak zone temperature	150–200°C
Time above liquidus (TAL)	30–100 s
Peak temperature	230–262°C
Cooling ramp rate	0.5–6°C/s

Source: Indium Corporation (2018). The above table is an adaptation of Indium Corporation, (2018)

Figure 11 The ramp/soak/spike profile of Sample 1

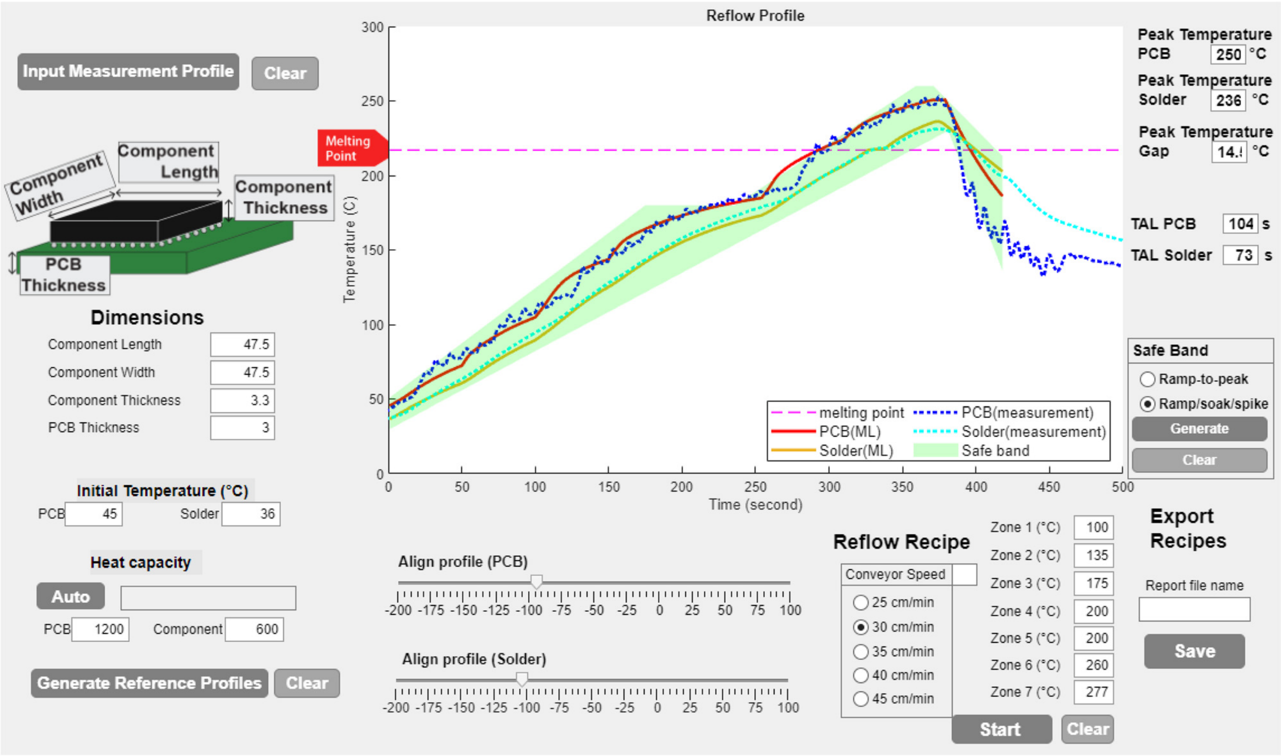

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Figure 12 The ramp-to-spike profile of Sample 2

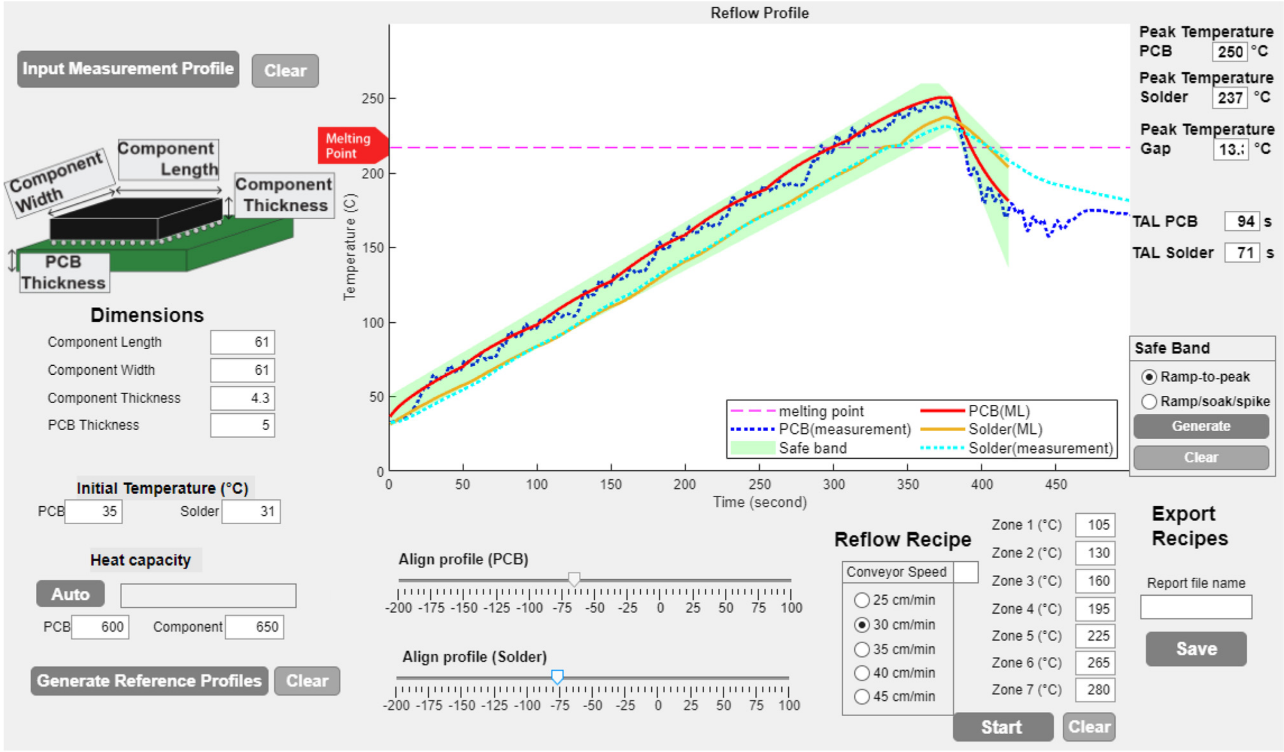

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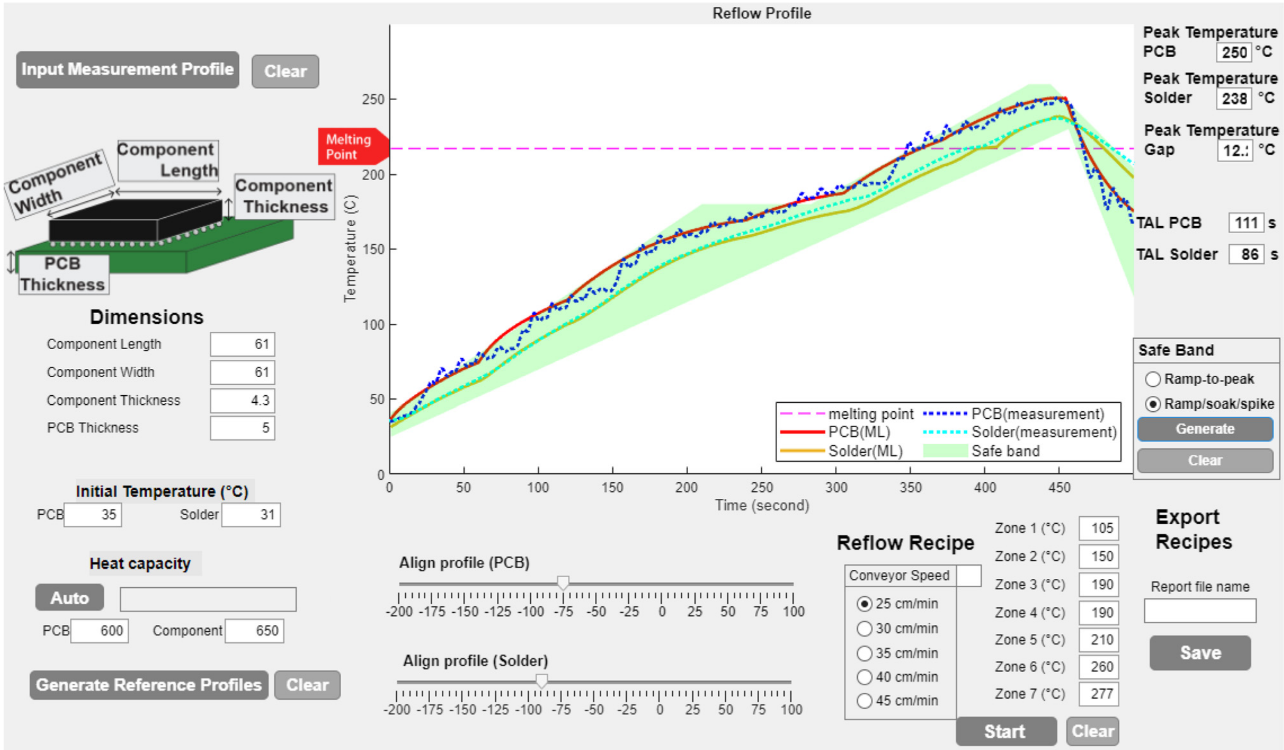
Figure 13 The ramp/soak/spike profile of Sample 2



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component's structure. ML algorithms were used to interpolate sparse data and provide speedy responses with RMSE below 0.1. This proposed approach effectively tackles optimization problems that involve multiple factors.

The development of the reflow recipe generator involved combining the CFD model and ML model to facilitate reflow profiling via a user interface. The heat capacities of the assembly, which are the unknown valuables, can be determined inversely by using a series of experiment results. The trained Gaussian process regression models are then used to perform virtual reflow profiling. Upon ensuring that the resulting profiles are inside the safe zone, the corresponding reflow recipes can be used to configure the reflow oven. Instead of relying on field measurement completely, this approach greatly decreases time and labor costs in trial and error.

It is important to note that the ML models are specific to the oven in use. Therefore, if the model is intended to be used with other ovens, it is necessary to perform validation for CFD models and generate training data again in accordance with the instructions outlined in the paper.

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