How AI can Accelerate R&D for Solder Paste Formulations

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ABSTRACT
Solder pastes formulations constantly encounter new challenges such as the incorporation of new alloys, the refinement of powder granulometry, reduction of voids, and mitigation of residue corrosion. Each solder paste must adhere to certain minimum specifications, including solderballing, low slump, and wettability, regardless of its intended application. When developing new formulations, approximately fifteen ingredients are adjusted or created to meet these specifications. Due to the complexity of the formulations, the studies are time-consuming. However, the use of new methods based on Artificial Intelligence (AI) enables optimizing the composition of solder paste with specific properties and cutting development times by drastically reducing the number of tests to be carried out.

As a field of research, the full understanding of the factors influencing formulated products remains incomplete and the scientific literature about this topic is scarce. To address this problem, AI is proving capable of going beyond human detection of correlations between the features of a phenomenon [1]. Our focus lies in leveraging AI to predict the key solder paste properties to comply with new market specifications and exploring the potential for generating new formulas. This resulted in the testing of hypotheses and the development of a solution, harnessing the efficiencies offered by AI in reducing both time and resources during the formulation development phases of solder paste.

In conclusion of this article, a comparison is made between the experimental results and the AI anticipated results. Analyzing these results in alignment with the methods used in data science not only advocates for the significance of experimentation in AI but also enhances the agility of AI project, particularly in the field of solder paste applications and broader chemicals.

Key words: AI, prediction, characteristics, formulation, solder paste.

INTRODUCTION

Formulation challenges [2] [3]

A solder paste is made of a metallic part and a flux medium, the latter being made up of different ingredients: activators, resins, thixotropic agents, and solvents. Each of the ingredients plays a role in the final characteristics of the solder paste.

The flux medium is the vehicle of the alloy powder; it provides viscosity and rheology, eliminates oxides films on substrates, protects the powder from oxidation and reduces the surface tension of the alloy during reflow to enhance wettability. A flux medium contains several kinds of ingredients:

- Resins

Synthetic resins can be used, but most resins used in solder pastes are in fact rosins, based on colophonium derivatives. These rosins mainly act as binders in the formulation. Most rosins are acid by nature and are characterized by an acid index which indicates the quantity of acid contained in a substance: rosins partially play the role of activators. Generally, to get the best performance, a mix of several rosins is used.

- Activators

Activators remove oxide from the metallization and the powder to promote the solderability. Weak organic weak acids are the most used, and halogens if permitted. Acids are characterized by a melting point, a boiling point, sometimes a decomposition temperature, a solubility level in different solvents and are often used in combination with an amine. In general, if the acids have a short chain, the efficiency is high (higher acid index) when short reflow profiles are used but the stability of the solder paste is less: these acids tend to react at a too low temperature (i.e. room temperature). Fatty acids are not strong activators but are able to stand higher temperatures; they are easier to dissolve in non-aggressive solvents than the shorter acids. Additionally, they may stabilize the formulation.

- Solvents

Solvents dissolve the ingredients of the flux medium such as rosins and activators. Solvent with rather high boiling point, usually above 200°C, are mainly used in lead-free solder pastes. The solvents are characterized by their solvency power, viscosity, surface tension, boiling point, vapor pressure, polarity, etc. The choice of suitable solvents is a key factor for preheat and reflow properties as well as for the stability and printability.

- Thixotropic agents

Thixotropic agents are used to stabilize the flux medium and to bring the desired rheology.

- Additives

More and more additives are added in the flux medium: plasticizers, antioxidants or preservatives.

For the development of new formulations, a recipe of around fifteen ingredients is modified or invented to meet the required specifications. Each ingredient is used in a specific proportion to give the best performance from the solder paste. The formulator must consider the solubility of the ingredients, their action in the final application and the interactions they can have between each other's.

Every project generates multiple formulation possibilities with the associated characteristic tests. As beyond a dedicated requirement, a solder paste must meet the basic and key performances related to the electronic application. The studies are time-consuming due to the complexity of the formulation. However, the use of new methods based on Artificial Intelligence (AI) enables optimizing the composition of solder paste with specific properties.

AI as a tool for solder paste formulations

Artificial intelligence and machine learning techniques offer promising new approaches to accelerate research and development of solder paste formulations. By leveraging large datasets of material properties and performance characteristics, AI models can rapidly explore the vast design space of potential solder paste compositions. Machine learning algorithms can identify complex patterns and relationships between ingredients, process parameters, and paste properties that may not be readily apparent to human researchers. This data-driven approach allows for more efficient screening and optimization of novel formulations, potentially reducing the time and cost of traditional trial-and-error experimentation. As AI capabilities continue to advance, integrating these tools into the R&D workflow could significantly speed up innovation cycles for next-generation solder pastes.

Building upon the AI-driven approach to solder paste formulation, the next crucial step involves a meticulous evaluation of data quality, a factor that profoundly impacts the reliability of subsequent analyses and predictions. This evaluation is formalized through the implementation of a confidence index, a metric that quantifies the robustness of the dataset by considering multiple factors, including the proportion of missing data and the uniformity of data distribution across various parameters. Extensive testing has revealed that a homogeneous distribution of values across the dataset is highly desirable, as it ensures that the AI model is trained on a diverse and representative range of solder paste compositions and properties. This approach significantly enhances the model's ability to generalize its predictions accurately, even when faced with novel formulations or manufacturing conditions. The next step of the method is based on training a supervised machine learning model, as illustrated in Figure 1.

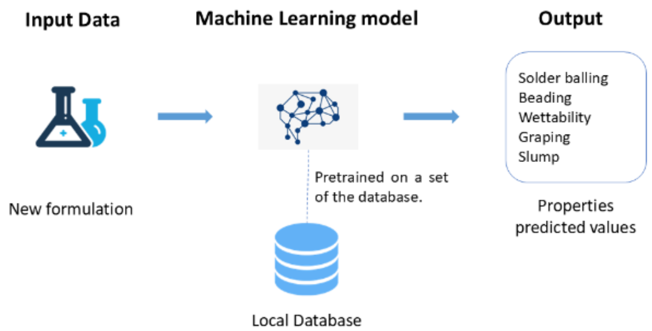


Figure 1: Machine learning process

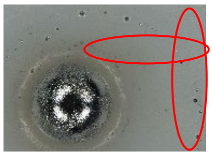
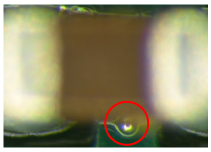
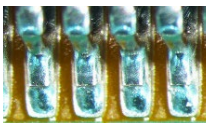
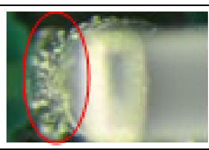
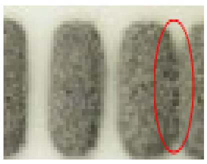
The diagram describes a supervised learning process. The model is trained using a local database from the R&D department and is designed to predict the properties of a new formula by examining its composition and the correlations between compositions and tests. This innovative process marks a substantial improvement in both efficiency and precision in the creation of new formulas.

After this introduction a short description of the typical tests to describe solder pastes characteristics and properties is shared. Then the AI approach to predict these characteristics and properties is explained. To complete the study, a case study is described as results showing the concrete possibilities of the model. The main outcomes are summarized in the conclusion.

SOLDER PASTE CHARACTERISTICS

The characteristics listed below in Table 1. are the key properties for every new developed solder paste regardless of the specific requirements. These are properties that all solder pastes must satisfy. Other characteristics are also important such as rheology, viscosity or cleanability, but these latter characteristics depend on the final application of the product. Our method focuses solely on requirements that are common to all solder pastes developed. It should be noted that all our solder pastes used in this study are SAC305 based.

Table 1: Solder paste characteristics description

Characteristic	Description	Picture
Solderballing	stuck microballs after reflow around pitch lands and solder mask	
Beading	trapped solder balls under or next to chip components	
Wettability	ability of molten solder paste to bond with the substrate and the component	
Graping	unreflowed solder particles on top of the solder reflow deposit	
Slump	solder paste spreading during preheat	

To evaluate the various characteristics presented in Table 1, we have defined specific test methods:

- Solderballing

The solder paste is printed on the alumina substrate. Alumina substrates are reflowed (at 250°C) with seven preheat conditions.

The marking is done after binocular inspection, magnification x30, according to the following:

Class 1: 5 solderballs maximum
Class 2: 6 to 10 solderballs
Class 3: 11 to 20 solderballs
Class 4: 21 to 50 with possibility of a slight lisere
Class 5: More than 50 solderballs with clusters and lisere

➢ Beading

Using a FR4 copper test board, the paste is printed on the 0201 design, chips are placed and reflowed using a standard linear reflow profile. After reflow an observation of potential stuck micro balls is done under microscope. This is a pass/fail test.

➢ Wettability [4]

The following test method is mainly based on IPC-TM-650 2.4.45 and adapted to our specifications. The solder paste is printed on the copper substrate. Copper coupons are reflowed (at 250°C) with four preheat conditions.

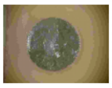
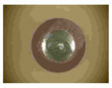
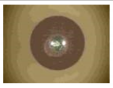
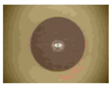
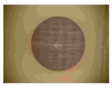
The marking is done after binocular inspection, according to the following:

Class 1: solder spreads more than printed area
Class 2: solder spreads equal to printed area
Class 3: solder spreads less than printed area or evidence of dewetting or non-wetting

➢ Graping

The solder paste is printed on a FR4 copper substrate with specific openings as seen in the Table 2 below.

Table 2: Graping test stencil apertures

Print Deposit (mm)				
5.00	3.00	1.00	0.60	0.30
				

Two reflow profile per paste are tested: a standard linear reflow profile and a soak reflow profile. After reflow, the presence of graping is checked for each deposit.

➢ Slump [5]

The solder paste is printed on alumina substrates through the IPC-A21 0.2mm thick stencil. Hot slump is done by preheated the substrate for 15 minutes at 180°C and then cooled to ambient temperature. The number of bridges is counted between all deposits (Figure 2).

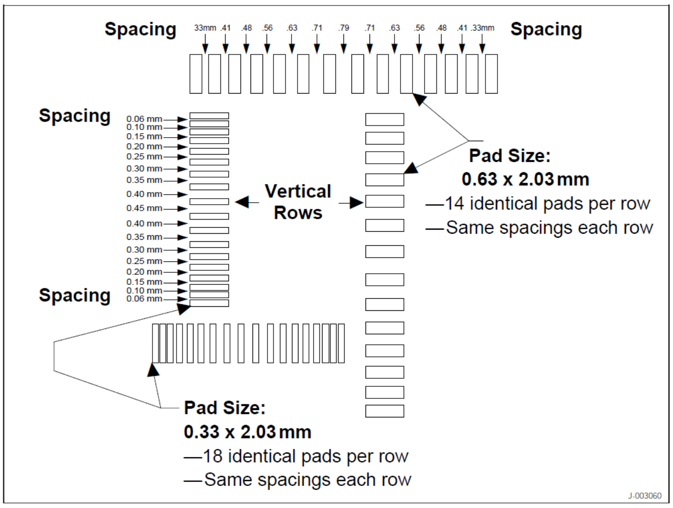


Figure 2: Slump design IPC-A21

The aim of the research is to use the key characteristics as output data for the AI to make an initial selection of the formulations to be chosen as part of the development of a new paste. The following Table 3 summarizes our test classification, the type of data it generates for the AI and our acceptance criteria (based on our experience in the electronic industries as basics to fulfill).

Table 3: Characteristics classifications

	Type of Data	Classification	Inventec criteria of acceptance
Solderballing	Numerous	Sum of the classes counted	<10 Pass >10 Fail
Beading	Categorical	1= no solder beading 2= solder beading	1 Pass 2 Fail
Wettability	Categorical	1= Class 3 with solder projections 2= Class 2 with a lot of microballs 3= Class 2 with some microballs 4= Class 2 without microballs	1&2 Fail 3&4 Pass
Graping	Categorical	1= graping with both reflow profiles 2= graping with one reflow profile 3= slight graping with one reflow profile 4= no graping	1&2 Fail 3&4 Pass
Slump	Numerous	Sum of the bridges	<28 Pass 28<x<36 Acceptable >36 Fail

The data that will be generated from all formulations tested, will be used to feed the AI. The use of AI to predict the results for each characteristic will be detailed, as will the obtained performance prediction. By integrating these AI-powered predictions into the R&D workflow, we aim to significantly reduce the number of experimental iterations required to achieve optimal formulations.

Through this research, we seek to establish a new paradigm in materials science R&D, where AI serves as a powerful tool to augment human expertise, leading to faster innovation cycles, reduced costs, and the development of next-generation solder pastes tailored to meet the ever-evolving demands of modern electronics manufacturing.

AI APPROACH

For our solder paste formulation use-case, the Gradient Boosting Decision Tree (GBDT) model emerges as a particularly suitable choice, offering impressive performance metrics.

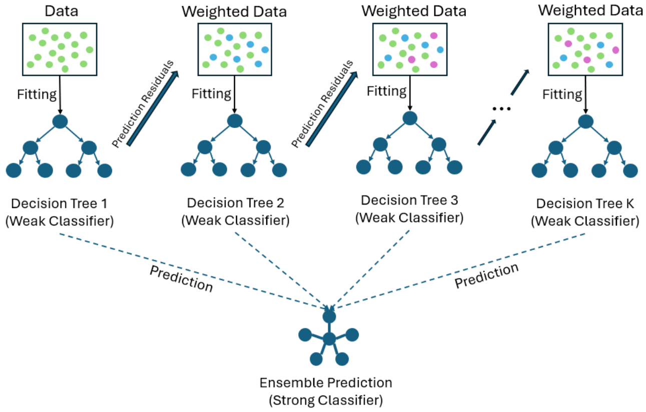


Figure 3: The architecture of a Gradient Boost Decision Tree model

This advanced machine learning algorithm, a member of the ensemble methods family, iteratively constructs a series of decision trees, with each subsequent tree fine-tuning the predictions of its predecessors. GBDT distinguishes itself from conventional boosting techniques by employing gradient descent optimization to minimize a defined loss function. During each iteration, the algorithm adeptly fits a new decision tree to the negative gradient of this loss function, effectively learning from the residuals of prior predictions.

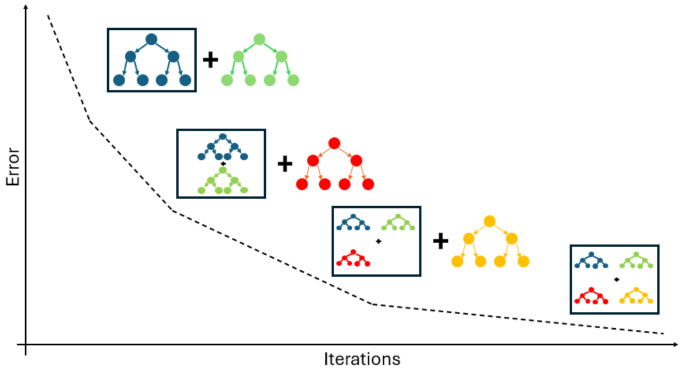


Figure 4: How GBDT reduces errors after every iteration

This sophisticated approach enables GBDT to adeptly navigate and model the complex, non-linear relationships inherent in solder paste data with remarkable accuracy. The model's versatility is evident in its applicability to both regression and classification tasks, making it well-suited for various aspects of solder paste analysis. In the specific context of solder paste formulation, GBDT excels at capturing the subtle and intricate interactions between diverse ingredients and process parameters. This capability positions GBDT as a powerful tool for generating more precise predictions of crucial paste properties and performance characteristics, potentially accelerating the R&D process and leading to innovative formulations.

The primary focus of this study is using AI to enhance solder paste formulation processes. In conventional methods, approximately 20 potential formulas were developed to meet customer requirements. The objective of implementing AI is to streamline this process by decreasing the number of candidates, thereby enabling tests to be conducted on only the three most promising formulations.

RESULTS

Data accuracies

Following the various experiments carried out in our laboratory to predict the test properties for the formulations, several interesting observations led to the resolution of certain problems and the emergence of ideas for testing. As depicted in Table 4 below, the predicted characteristics values accuracies were determined based on the outcomes of the performed experiments.

Characteristic	Accuracy
Solder balling	75%
Beading	98%
Wettability	97,50%
Graping	99%
Slump	95%

Table 4: AI characteristics prediction accuracies.

The accuracy is noticeably superior for properties that possess categorical data type, such as Graping and Wettability. This metric exhibit improvement with an increase in the quantity and quality of data. However, a point can be reached where the enhancement in accuracy is minimal compared to the effort invested in gathering and processing data.

The experiments were performed using various sizes of the database: one with minimal but quality data, another with the maximum possible data entries, and the last one with a reasonable quantity of complete data.

The results of these experiments underscore the benefits of prioritizing data completeness (minimal missing values) over the number of formulations with incomplete tests. A smaller dataset devoid of missing values offers more valuable insights for the model than a larger dataset with an abundance of missing values.

Deduction of raw materials impacts

The experience and expertise of the R&D teams enable the deduction of the various impacts of the raw materials on the final characteristics. The know-how is reproduced and improved by AI Models like Gradient Boosted Decision Trees. This model calculates feature importance by measuring how much each feature contributes to reducing the loss function across all trees in the ensemble. For each feature, the algorithm sums the reduction in loss (or improvement in the splitting criterion like Gini impurity) whenever that feature is used for a split. Features that are used more frequently for important splits (those that significantly reduce the loss) are deemed more important. The total gain for each feature is then normalized to get relative importance scores, typically expressed as percentages.

For our specific knowledge domain, AI helped summarizing raw materials influence on solder paste characteristics:

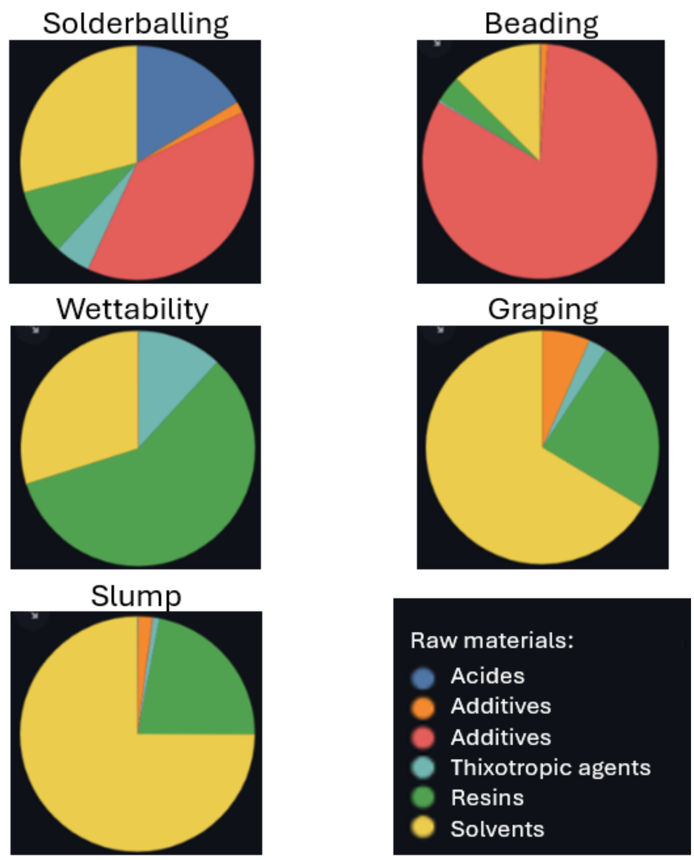


Figure 5: Raw materials influences on solder pastes characteristics

Figure 5 shows the impact of the raw materials on the key characteristics of solder paste. Some of these results were already known from the literature or from our own experience. What is interesting to note, however, is the difference in the magnitude of the impact from one type of raw material to another. For example, solvents for slump or additives for beading have a major impact on the results of these tests. AI also allows us to go further and give us details by specific raw material, which we are not revealing here for obvious reasons of confidentiality.

CASE STUDY

Context and requirements

At the start of each project, a set of specifications is defined, based on which we assess the formulation possibilities. The formulations are defined according to the specific characteristics required, using new raw materials or changing the proportions of existing raw materials. These modifications to the formulations must complement the specific characteristics of the requirements but must not degrade the basic and key characteristics that a solder paste must respect (solderballing, wettability, slump, graping, beading).

In the specific case of this study, the customer concerned wants a solder paste that limits the clogging of the reflow oven; this means that the cleaning frequency of the oven is too high for their process. In fact, the ovens used in assembly processes become clogged due to the evaporation of solvents polluted by the residues that make up the flux of soldering paste.

R&D analysis (DOE, formulation screening)

Initially, the R&D team had to identify the raw materials responsible for the phenomenon observed by the customer (clogging of the oven). Following this study, it was identified that the solvents and resins used would have the greatest impact on the problem observed. The pollution and the clogging of the ovens is the logical consequence of the evaporation of solvents polluted by the resins contained in the flux medium.

Several possible formulations have been put forward based on this latest status of the raw materials responsible for pollution in reflow ovens. These formulations use different proportions of resins and solvents to reduce the evaporation of polluted solvents in the ovens. The main factor sought for solvents is their boiling point, while for resins it is interesting to vary their solubilizing power in the solvents.

This research analysis produced 21 possible formulations. These formulations will be analyzed by the AI so that it can deduce the results for the various basic characteristics (solderballing, beading, wettability, graping, slump).

AI analysis

The following Table 5 shows the AI predicted results for the various characteristics (solderballing, beading, wettability, graping and slump). Results with a green color are those within the acceptability criteria, orange are out of specification and yellow are within the acceptability limit.

Table 5: AI predictions of the characteristics results

Formulations	Solderballing	Beading	Wettability	Grapping	Slump
	Total of 7 conditions	1 = pass 2 = fail	4 & 3 = pass 1 & 2 = fail	4 & 3 = pass 1 & 2 = fail	Number of bridges
1	13	2	3	3	9
2	12	2	1	3	30
3	9	1	4	3	20
4	12	2	1	2	30
5	12	2	1	3	27
6	12	1	3	4	25
7	7	1	1	4	20
8	9	1	1	4	18
9	9	1	4	3	21
10	12	2	1	2	32
11	11	2	1	3	27
12	9	1	1	4	19
13	7	1	3	3	18
14	9	2	1	3	32
15	10	2	4	2	26
16	10	2	2	3	45
17	12	1	3	3	29
18	10	1	3	3	12
19	12	1	3	3	16
20	11	1	3	3	30
21	8	1	1	3	33

The results predicted by the AI enable to identify 4 formulas that have satisfactory basic characteristics for this project. Formulas 3, 9, 13 and 18 show results within the given acceptance criteria.

Initially, the data obtained by AI prediction is reproduced in the R&D laboratory to confirm the obtained values.

A comparison of the predicted results and the analyzed results is shown in Table 6:

Table 6: Comparison of predicted and analyzed results

Formulations		Solderballing	Beading	Wettability	Grapping	Slump
		Total of 7 conditions	1 = pass 2 = fail	4 & 3 = pass 1 & 2 = fail	4 & 3 = pass 1 & 2 = fail	Number of bridges
3	Predicted	9	1	4	3	20
	Analyzed	10	1	4	4	16
9	Predicted	9	1	4	3	21
	Analyzed	9	1	4	3	29
13	Predicted	7	1	3	3	18
	Analyzed	8	1	3	3	23
18	Predicted	10	1	3	3	12
	Analyzed	9	1	4	3	16

The first conclusions that can be drawn from this comparison between the experimental results and the AI predictions is that most of the results are very close to the predictions. Only one slump result for formula 9 pushed the paste in the limit of acceptability.

This is one of the reasons why AI is useful in helping us to select the best formulas for a screening or DOE, but it is useful to reconfirm the experimental tests on the selected formulas, which already reduces the amount of testing to be carried out.

Fulfill the specific requirements

Now that the results of the characteristic tests on the selected formulas have been validated, R&D team needs to go back to the customer's specific specifications, i.e. a solder paste that limit the pollution of reflow ovens. To achieve this, a new laboratory test is developed, the test simulates the quantity of residue that would remain trapped in the oven and cause the pollution over the long term. The test consists, as shown in the Figure 6, using crystallizers, to entrap the residues droplets appearing during the reflow process (due to solvent evaporation polluted by resins).

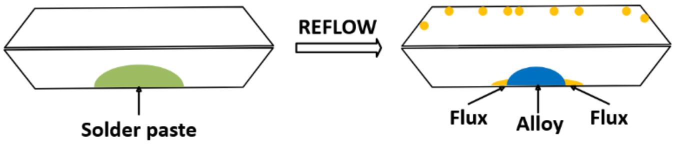


Figure 6: R&D test schema

After reflow, and a given time, a weight is done on the top crystallizer. A high weight in the top crystallizer means that there is a high potential of pollution. In the Table 7, the weight results of the top crystallizers are shown for the 4 formulations and a reference that pollutes the ovens of the customer. The new formulations can be evaluated in comparison the reference and check the improvements.

Table 7: Test results – quantity of trapped residues

Formulations	Weight of the top crystallizer (g)					
	Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Average
Reference	1,1302	1,1316	1,1309	1,1297	1,1301	1,1305
3	1,1932	1,1925	1,1926	1,1930	1,1929	1,1928
9	0,9187	0,9185	0,9181	0,9179	0,9189	0,9184
13	1,0785	1,0782	1,0791	1,0779	1,0780	1,0783
18	0,9365	0,9359	0,9367	0,9371	0,9374	0,9367

The test has been done 5 times with each formulation to confirm the repeatability of the test. The repeatability is confirmed, and the results can be analyzed.

Of the 4 formulations analyzed, 3 have lower top crystallizer weights. They are therefore less likely to cause pollution in the reflow ovens. Formula 3 gave a higher result than the reference. Formula 3 was therefore not selected for further analysis.

Other specific characteristics were analyzed for the 3 remaining formulations (9, 11 and 18), such as screen printing, viscosity, rheology and cleaning. The 3 remaining formulations showed satisfactory results for the latter tests.

AI enabled us to select 4 of the 21 formulas proposed by the R&D team, considering the know-how and impact of the raw materials on the requested specifications. Specific tests were carried out on the remaining 4 formulas to select the best formulation to offer the customer. Formula 18 was chosen because it was the formula with the best performance between the specific and the basic characteristics. Formula 18 will therefore be sent and tested by our customer.

CONCLUSION

In this study, AI was used to predict the results of the key characteristics to better select the choice of formulas, to understand the relationship between molecules and to spend time on other aspects of the developments (specific requirements, processes, etc.). To be able to exploit AI data in a relevant way, we highlight that the input database itself is crucial to generating reliable output data. A great deal of work needs to be done upstream on data relevance before AI capabilities can be exploited.

As part of the development of a new solder paste formulation, AI made possible to:

- improve the relevance of the selected formulas,
- limit the time spent on manufacturing formulations and carrying out tests,
- reduce consumption of raw materials and consumables.

AI is also helping to increase our knowledge of the interactions between raw materials and their impact on the various characteristic tests.

The use of artificial intelligence is a great opportunity to improve the efficiency and relevance of the projects we monitor. It is important to note that AI is a tool, not a replacement for a high-performance R&D team with strong know-how.

In the near future, AI could be used to predict the behavior of soldering pastes by varying the alloys used. This perspective is also in line with the objective of saving time and improving efficiency.

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