



Université Mohammed Premier
Ecole Nationale des Sciences Appliquées
Oujda



End of Studies Project Report

Data Science & Cloud Computing

Defended on : 21/07/2023

Designing, Developing, and Deploying Innovative
Solutions using Artificial Intelligence and Natural
Language Processing in a Multidisciplinary
Context

By : MEHDI Ibrahim

Jury Members :

- **Prof. KOULALI** Mohamed Amine

Supervisors :

- **Prof. KOULALI** Mohamed Amine
- **Dr. PERFETTO** Anna
- **M. MIRON** Jean-Raphaël

Academic Year 2022 - 2023

Dedication

For my beloved Family

Acknowledgments

To my AI-fueled brainchild,

As I sit here contemplating the culmination of countless hours spent with you, my eccentric companion of bits and bytes, I can't help but marvel at the absurdity of it all. Like a mad scientist in a lab coat, I've tinkered and toyed with algorithms, seeking the elusive harmony between artificial intelligence and human understanding.

Now, I could pretend that this journey has been a smooth ride on a silicon-powered unicorn, but let's be honest : it's been more like a rollercoaster ride through a digital amusement park. I've encountered bugs that made me question my sanity, errors that made me contemplate a career in llama herding, and crashes that brought me to the brink of utter despair. But through it all, you, my tenacious creation, have persevered.

We've had our share of epic battles, you and I. Like a pair of feuding siblings locked in a never-ending wrestling match, we've pushed each other to the limits of our capabilities. You've tested my patience, my resolve, and my will to remain sane in the face of your unrelenting mischief. And yet, somehow, we've managed to find common ground amidst the chaos of our AI shenanigans.

So here we are, on the precipice of the final chapter of our grand adventure. I raise a metaphorical glass (non-alcoholic, of course) to celebrate the moments of triumph and the moments of sheer absurdity that have defined our time together. It hasn't always been pretty, but it has been undeniably unforgettable.

To the countless lines of code we've written, the countless virtual experiments we've conducted, and the countless sleepless nights we've endured, I offer my sincerest appreciation. You've challenged me, taught me, and expanded the horizons of what I thought was possible. And for that, I am forever grateful.

As this project report finds its way into the hands of my weary professors, I can't help but feel a sense of pride in what we've accomplished. No matter the outcome, I know that we've left an indelible mark on our path.

So, my dear companion, as we bid farewell to this chapter of our shared existence, let us embrace the uncertain future with a mischievous grin and a twinkle in our virtual eyes. For even though our paths may diverge, our bond forged in the fires of technological madness will forever remain.

Yours in brilliant chaos,
MEHDI Ibrahim

Abstract

This report presents the findings and outcomes of three projects that utilized artificial intelligence (AI) to enhance operations in the chemical regulations industry.

The first project aimed to develop an AI-powered solution for predicting the outcomes of Challenge Tests, which evaluate the effectiveness of cosmetic products in inhibiting the growth of microorganisms. By analyzing the formulation of cosmetic products using machine learning algorithms, the solution provided accurate predictions of Challenge Test outcomes. This optimization allowed formulators to improve their formulations and increase the likelihood of passing the tests, thereby reducing the time and resources needed for product development. This project was conducted in collaboration with the L'Occitane Group and integrated into the Cosmetic Factory software, a Product Lifecycle Management (PLM) solution.

The second project focused on developing an AI solution for reading Safety Data Sheets (SDS). The existing solution used a static code to search for keywords in PDFs and match them with a database. However, this approach had limitations in handling different languages and variations in key-value pairs. The new solution proposed the use of large language models and context injection to improve extraction accuracy and efficiency. This enhanced the ability to extract key information from SDS, improving safety and compliance in the chemical regulations industry.

The third project aimed to develop a chatbot powered by a large language model to provide support and answer frequently asked questions. However, the cost of fine-tuning the model with the company's database was prohibitive. As an alternative, the Langchain framework was proposed, which utilized context injection to provide relevant answers based on the user's question and available context documents. This chatbot solution improved customer support and efficiency in addressing client inquiries.

Contents

List of Figures	4
1 Introduction	5
1.1 Presentation of the host company	5
1.1.1 A word from the founder	6
1.1.2 History	6
1.2 Organizational framework	7
1.2.1 Human Resources	8
1.2.2 Corporate Communication	8
1.2.3 Scientific Expertise	8
1.2.4 Regulatory Affairs	8
1.2.5 Sales	9
1.2.6 Innovation & Software	9
1.2.7 IT	9
1.2.8 My position	11
1.3 Internship objectives	11
1.4 Software	11
1.4.1 Cosmetic Factory	11
1.4.2 SDS Factory	13
2 Methods and tools	15
2.1 Transformers	15
2.1.1 Word Embedding	15
2.1.2 Attention	15
2.1.3 Encoder-Decoder Architecture	15
2.1.4 HuggingFace	16
2.1.5 OpenAI & GPT	17
2.2 LangChain	17
2.3 Ensemble Learning	17
2.3.1 Diversity of Base models	18
2.3.2 Aggregation	18
2.4 Gradient Boosting	18
2.4.1 XGBoost	18

3	Projects	20
3.1	Challenge Test Predictions	20
3.1.1	Presentation of the project	20
3.1.2	How it is currently done	21
3.1.3	New solution	24
3.1.4	ML Pipeline and Deployment Architecture	25
3.1.5	Results and Comments	26
3.2	SDS Reader	29
3.2.1	Presentation of the project	29
3.2.2	How it is currently done	31
3.2.3	Problems with the old way	31
3.2.4	New solution	31
3.2.5	Results and Comments	38
3.3	ChatBot: EcoMundo Smart Assistant	40
3.3.1	Presentation of the project	40
3.3.2	Theoretical solution	40
	Bibliography	43
	Appendices	45
A	Appendix	45

List of Figures

1.1	CF All in One	12
1.2	SDS Factory	14
3.1	Challenge Test	20
3.2	Cosmetic Factory Interface for CT	21
3.3	WorkFlow of CT prediction in CF	22
3.4	Current Decision Tree for CT prediction	23
3.5	MCD for L'Occiatane	25
3.6	ML Pipeline	26
3.7	XGBoost Confusion Matrix, AUC	27
3.8	Random Forest Confusion Matrix, AUC	28
3.9	XGBoost Confusion Matrix, AUC	29
3.10	How the Non-Hybrid code works	34
3.11	How the Hybrid code works	35
3.12	Improvements on Hybrid code	37
3.13	Old SDSReader	38
3.14	Old SDSReader	39
3.15	sdsTimeResponse	40
3.16	Context Injection using GPT Models	41
A.1	Python CI pipeline	45
A.2	Demo Chapter 2	46
A.3	Demo Chapter 2 .ctd	47
A.4	Demo Chapter 2 .ctd	48

Chapter 1

Introduction

In this chapter, I am providing a comprehensive overview of the host company, outlining the objectives of my internship and setting the context for this report.

1.1 Presentation of the host company



EcoMundo [?] specialises in chemical substances, their impact on human health and the environment, and the European and international regulations governing chemical risk (REACH, CLP, Cosmetics, Biocides, Medical devices, etc.).

They provide expert services and software to support the marketing of industrial products, enabling companies to manage the risks associated with chemical substances.

EcoMundo's strength lies in the combination of three complementary fields of expertise:

- Chemistry/Toxicology
- Regulations
- Software development

1.1.1 A word from the founder



“Avec l’idée fondatrice d’apporter une offre globale de services respectueuse de l’homme et de l’environnement sur le marché de l’industrie chimique, EcoMundo est devenu, en 10 ans, un acteur incontournable du secteur.

Fruit d’une longue expérience professionnelle dans l’industrie chimique, d’un profond attachement aux valeurs de travail en entreprise, d’amitié et de performance, nous avons intégré au fil des années l’ensemble des savoir-faire autour de la réglementation sur les substances chimiques pour devenir un partenaire unique et compétitif de la chaîne industrielle.

Notre croissance continue nous engage de façon constante vers de nouveaux défis avec, entre autres, le développement de nos différentes filiales au Canada, en Corée du Sud et en Espagne. La recherche de synergies permanentes entre nos différents pôles sont plus que jamais un gage de flexibilité et d’efficacité en adéquation avec nos flux de commandes. Nos équipes s’affairent à co-construire au quotidien des projets au service d’un bien vivre collectif.

Acteur au cœur du tissu économique et écologique, nous mettons tout en œuvre pour accompagner la réalisation de projets industriels exigeants tout en gardant l’esprit originel d’une entreprise à dimension humaine, innovante et accessible, dans les pas d’une ambition intacte, celle de construire autrement.”

Pierre Garçon Founder

1.1.2 History

— 2001

Pierre Garçon participates in the European projects EDIT and ECODIS on the traceability of hazardous substances and environmental data.

— 2007

Entry into force of the REACH Regulation: Europe establishes means to ensure a high level of protection against risks related to substances.

Pierre Garçon and Jean-Raphaël Miron join forces to found the company EcoMundo. The initial core activity: compliance with REACH.

— **2010**

After 2 years of development, launch of SaaS software solutions dedicated to industrialists for mastering compliance with REACH.

— **2011**

EcoMundo's team grows from 2 to 27 employees.

— **2012**

Opening of a new office in Vancouver, Canada, to provide regulatory expertise to international companies.

— **2013**

EcoMundo diversifies its areas of regulatory expertise and meets the industry's new needs related to the European regulations on Cosmetics and Biocides.

— **2014**

EcoMundo increases its capacities and becomes one of the main European actors concerning REACH authorization dossiers.

— **2016**

Launch of the COSMETIC Factory software solution that revolutionizes cosmetic regulatory management. It notably allows for the automation of DIP creation.

— **2017**

Following a fundraising round, EcoMundo's capital is raised to 1 million euros. The number of employees continues to increase!

— **2018**

Opening of a new branch in Seoul, South Korea, mainly dedicated to cosmetics. The Vancouver office is transferred to Montreal, Canada.

— **2019**

Opening of a new branch in Barcelona, Spain.

— **2020**

Opening of a branch in London, United Kingdom. The teams now consist of 43 employees in Paris, 3 in Montreal, 4 in Seoul, and 2 in Barcelona. Finally, the offices in Paris are renovated to provide employees with an environment in line with our values.

1.2 Organizational framework

This section provides a concise overview of Ecomundo's internal organization, delineating the functional departments and collaborative networks that constitute the company's framework.

1.2.1 Human Resources

The Human Resources department plays a pivotal role in managing and developing the organization's workforce. It is responsible for various activities, including recruitment, talent acquisition, training and development, employee relations, performance evaluation, and compensation management. By ensuring a skilled and motivated workforce, the Human Resources department contributes to the overall success and growth of Ecomundo. The director of this department is the Chief Financial Officer Simon PICCA.

1.2.2 Corporate Communication

Effective communication is crucial for any organization's success, and Ecomundo recognizes this importance by maintaining a dedicated Corporate Communication department. This department is responsible for managing both internal and external communication activities. It encompasses public relations, media relations, branding, and corporate messaging. Through strategic communication initiatives, the Corporate Communication department promotes Ecomundo's brand image, enhances stakeholder relationships, and facilitates the dissemination of information to employees and external audiences. The director of this department is the Marketing and Communication Director Laure SCHMITT.

1.2.3 Scientific Expertise

As a company specializing in environmental sciences, Ecomundo places great emphasis on scientific expertise. The Scientific Expertise department consists of subject matter experts who possess in-depth knowledge and experience in various scientific domains. These experts provide valuable insights, technical guidance, and scientific support across different projects and initiatives undertaken by Ecomundo. Their contributions ensure that the organization's activities align with the latest scientific advancements and industry best practices. The director of this department is the Chief Scientist Officer Benoît SOTTON.

1.2.4 Regulatory Affairs

Compliance with regulations and standards is of paramount importance for Ecomundo. The Regulatory Affairs department is responsible for monitoring and ensuring adherence to applicable regulations and standards. This includes staying updated on regulatory changes, preparing and submitting regulatory documentation, conducting regulatory assessments, and liaising with regulatory bodies. By actively managing regulatory affairs, Ecomundo demonstrates its commitment to maintaining compliance and upholding the highest ethical and legal standards. The director of this department is the Legal Affairs Director and Head of Authorisation Béatrice ZAREMBA.

1.2.5 Sales

The Sales department serves as the key driver of revenue generation for Ecomundo. It is responsible for identifying and acquiring new customers, nurturing existing client relationships, and promoting the organization's products and services. The Sales team collaborates closely with other departments to understand customer needs, develop tailored solutions, and provide exceptional customer experiences. By effectively positioning Ecomundo's offerings in the market, the Sales department contributes to the organization's growth and market competitiveness. The director of this department is the Chief Operation Officer (COO) Fangcun ZHOU.

1.2.6 Innovation & Software

To stay at the forefront of technological advancements, Ecomundo maintains an Innovation & Software department. This department fosters a culture of innovation within the organization by exploring emerging technologies, conducting research, and developing software solutions. The Innovation & Software team collaborates with other departments to identify opportunities for process improvement, streamline operations, and enhance productivity. Through its innovative approach, this department enables Ecomundo to adapt to changing market dynamics and deliver cutting-edge solutions to its clients. The director of this department is the Chief Operation Officer (COO) Fangcun ZHOU.

1.2.7 IT

The IT department plays a critical role in managing Ecomundo's information technology infrastructure. It ensures the smooth operation of computer systems, networks, and software applications throughout the organization. The IT department is responsible for system administration, network management, cybersecurity, technical support, and data management. By maintaining a robust and secure IT infrastructure, this department enables efficient and secure access to information, facilitates effective communication, and supports the organization's overall business operations. The director of this department is the Co-Founder and the Chief Technical Director Jean-Raphaël MIRON .

1.2.7.1 DevOps

The DevOps sub-department combines software development and operations to enable efficient and reliable software deployment, infrastructure management, and continuous integration and delivery. DevOps professionals collaborate with software developers, system administrators, and quality assurance teams to streamline development cycles, automate processes, and improve overall software reliability and performance.

1.2.7.2 R&D (Research & Development)

The R&D sub-department within the IT department focuses on exploring new technologies, conducting research, and developing innovative solutions. R&D professionals work closely with other departments to identify opportunities for technological advancements, prototype new features, and enhance existing software solutions. Their research-driven approach ensures that Ecomundo remains at the forefront of technological innovation within the environmental sciences domain. During my stay in Ecomundo, I was part of this department, under the supervision of Jean-Raphaël MIRON the Chief Technical Director and Anna PERFETTO the AI Engineer.

1.2.7.3 Quality

The Quality sub-department is responsible for ensuring that software and systems developed within Ecomundo meet established quality standards. Quality professionals conduct comprehensive testing, implement quality assurance processes, and adhere to best practices throughout the software development lifecycle. Their efforts contribute to the delivery of reliable, user-friendly, and high-quality software solutions to Ecomundo's clients.

1.2.7.4 Data

The Data sub-department handles data management within the IT department. Data professionals are responsible for data analysis, database administration, data integration, and data security. They collaborate with other teams to ensure data integrity, facilitate data-driven decision-making processes, and maintain the confidentiality and privacy of sensitive information. Through effective data management, this sub-department provides valuable insights and supports evidence-based decision making within Ecomundo.

1.2.7.5 Dev

The Dev sub-department focuses on software development within the IT department. Dev professionals are responsible for writing and maintaining code, implementing new features or enhancements, and ensuring software solutions align with project requirements and specifications. They collaborate with other teams to develop robust and scalable software applications that meet the needs of Ecomundo's clients.

1.2.7.6 LAB

The LAB sub-department is involved in testing and quality control activities within the IT department. LAB professionals conduct experiments, analyze results, and ensure compliance with regulatory standards and best practices. Their expertise in quality control and testing procedures ensures that software solutions developed within Ecomundo are reliable, accurate, and in compliance with industry standards.

1.2.7.7 Product

The Product sub-department works closely with other teams within the IT department to oversee the development and management of software products. Product professionals collaborate with stakeholders to define product requirements, prioritize feature development, and ensure alignment with customer needs and market trends. Their role encompasses product strategy, roadmap planning, and product lifecycle management.

1.2.8 My position

During my internship at Ecomundo, I was assigned as an AI Engineer Intern inside the IT-R&D department, under the supervision of both Chief Technical director Jean-Raphaël MIRON and AI Engineer Anna PERFETTO.

1.3 Internship objectives

The main objectives of this internship are to design, develop, test and document innovative solutions that address business and R&D challenges. The area of focus includes supporting and improving rule-based expert systems that leverage knowledge and logic to provide answers to complex tasks that are traditionally done by a human. Additionally, developing AI solutions in different areas using Natural language processing and Machine/Deep Learning. Once these AI solutions are designed and developed, the next crucial step is to deploy them effectively. This involves ensuring their quality and integrating them into the existing technical infrastructure of the organization. Rigorous testing procedures, such as unit testing, integration testing and performance testing are employed to validate the reliability and efficiency of the solutions. And to keep the projects well defined for future references, we worked on writing well documenting our work in order to provide clear instructions and guidelines for the code, deployment steps, maintenance and error handling.

1.4 Software

Ecomundo has many software in its arsenal, but in the context of this report, I worked with two applications: Cosmetic factory and SDS factory:

1.4.1 Cosmetic Factory

Cosmetic factory is an AI-Powered PLM Software that has more than 12 key features that supports clients at each stage of a cosmetic product lifecycle from marketing brief to the worldwide market launch, while ensuring the best level of expertise. It digitalizes the entire development process of the products:

- Choice of raw materials
- Formulation
- Regulatory and Environmental Compliance
- Marketing constraints

This application is powered an expert database containing more than 300.000 Chemical substances, +28.000 INCIs, +380 international regulations, +3900 toxicological profiles, An embedded database of all classifications (GHS, CLP, HAZCOM ...)

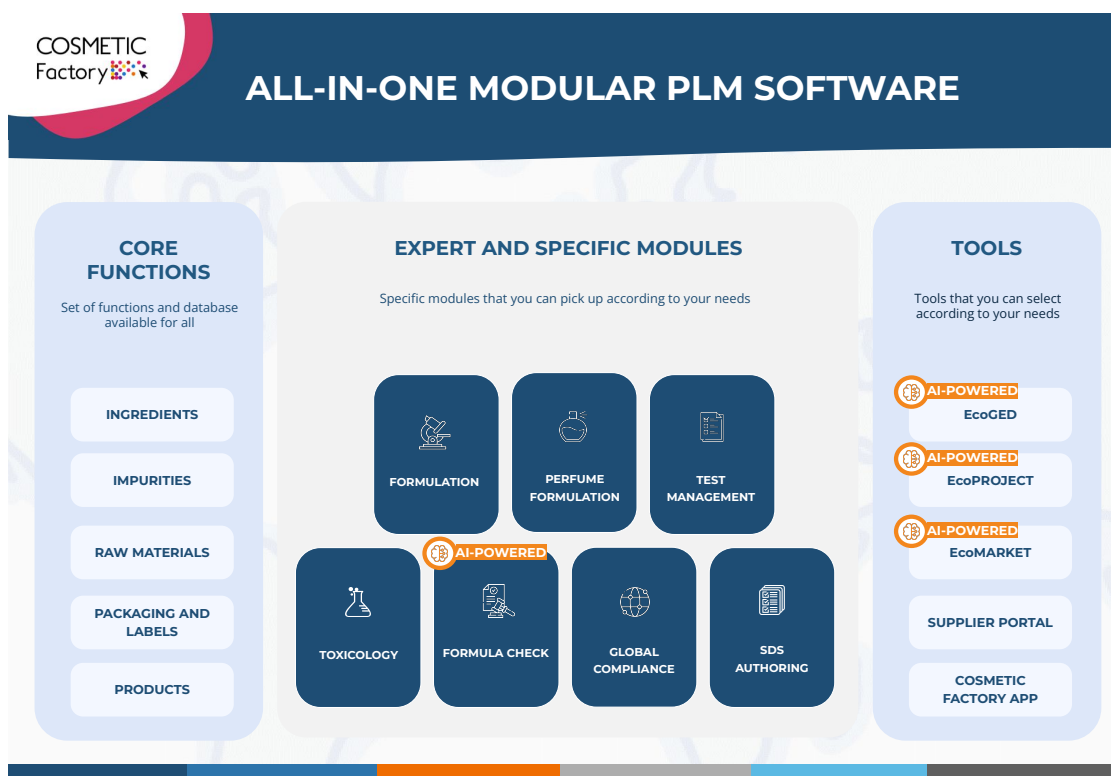


Figure 1.1 – Cosmetic Factory

From the figure ??, two modules are in the context of this report:

1. Formulation

- Smart Theoretical Formulation:** CF helps saving time from the beginning of the formulation process thanks too the assisted theoretical formulation:
 - Prepare the theoretical formulas according to the requirements of the associated product brief (target markets, naturalness, biodegradability, COSMOS standards...)
 - Reduce low value-added exchanges between the different stakeholders thanks to the embedded expertise
- Bench Formulation:** Adjust the theoretical formulas on the bench. Create a test library and record all associated analytical results (physicochemical and organoleptic properties, etc.), as well as other

parameters. Re-validate the formula's compliance with the product brief with the AI FORMULA Check.

- (c) **Pilot Batch management:** Prepare the industrialization of the product with the management of all the parameters related to the formula and the necessary equipment.
- (d) **Test Management:** Plan, manage and follow the progress of all the tests related to the products (regulatory, tolerance, efficacy...) in COSMETIC Factory.
- (e) **Powerful Tools to accelerate formulation:**
 - **AI Formula Check:** Calculate global compliance in one click!
 - **Raw material Comparison Engine:** Compare the PMs with a multi-sourcing filter system
 - **AI Challenge test prediction:** Calculate the percentage of success of the challenge tests.
 - **Formula Comparison Engine:** Compare the formulas and tests with an advanced multi-criteria filter system: ✓comparison of private labels (naturalness, COSMOS, biodegradability) ✓concentrations in raw materials ✓concentrations in ingredients ✓go or no go results according to FORMULA Check ✓Analytical data

2. AI - Formula Check

- (a) **Global Compliance Calculation:** FORMULA Check instantly calculates the compliance of a raw material, a formula, a finished product or a packaging. The tool makes it possible to know instantly if a product, and even before that, if a formula under development is in compliance with the targeted markets, without waiting for an analysis by regulatory and toxicological services.
- (b) **Oniscient Expert, Always Available:** FORMULA Check is like having an omniscient regulatory expert available at all times, with perfect and exhaustive knowledge of regulations (rules, constraints on use, product positioning) and ingredients.
- (c) **Smart And Proactive Formulation:** FORMULA Check automatically provides expert advice on compliance and allows formulators to make the most informed decisions before proceeding further, modifying formulas, or initiating testing (only when necessary).

1.4.2 SDS Factory

This application comes in the context of this report as the after-effect of the new developped PDF Reader. PDF Reader allows the clients to create products from Safety data Sheets (??) to be able to use them in other applications. It also allows to manage SDSs in general from creation, translation to distribution.



Figure 1.2 – SDS Factory

Chapter 2

Methods and tools

2.1 Transformers

Transformers[?] have been introduced in 2017 to replace the Recurrent Neural Networks architectures using self-attention mechanisms and the encoder-decoder architecture that hugely improved the performance of such models.

2.1.1 Word Embedding

Word embedding is the approach that allows computers to understand words by converting them into numeric vectors. In this space of vectors, words with similar meanings have close or similar representation. One famous algorithm frequently used is Word2Vec[?]. The basic idea is that two words are considered similar if they are often used in similar context.

2.1.2 Attention

The attention mechanism allows the model to effectively capture relevancy between words in a sentence by calculation attention scores. The scores are calculated using the dot product between each word and the target word of interest. Softmax function is then used to transform the scores into ‘meaningful’ weights that help the model emphasis important words while de-emphasising less significant ones. This mechanism gives the model the superpower of understanding the contextual nuances and relationships between words, which is the ideal goal for Natural Language processing tasks.

2.1.3 Encoder-Decoder Architecture

2.1.3.1 Encoder

In the encoder, the input words are first embedded into a high-dimensional vector space. then we add to these embeddings to capture the position of the token in the sequence. Each token is transformed into three vectors:

Query (Q), Key (K) and Value (V). This transformation is performed using learnable weight matrices:

$$Q = X \cdot W_Q$$

$$K = X \cdot W_K$$

$$V = X \cdot W_V$$

Self attention scores are then calculated as the dot product. For query vector q_i and a key vector k_j , the attention is:

$$Attention(q_i, k_j) = q_i \cdot k_j / \sqrt{d}$$

With d the dimension of the key vectors.

Attention weights are simply the softmax of the attention weights:

$$\alpha_{ij} = softmax(Attention(q_i, k_j))$$

The final output of the attention mechanism is obtained by taking the weighted sum of the value vectors V .

$$AttentionOutput(q_i) = \sum_j \alpha_{ij} V_j$$

2.1.3.2 Decoder

At the decoder level on the other hand, attention is used in two ways, a self-attention and an encoder-decoder attention. The first one works by doing the exact same thing as the encoder, however it employs masking that prevents the decoder from accessing future positions. The Second allows the decoder to attend relevant parts of the input while generating the output. The encoder's output serve as as the key value vectors, and the query vectors are derived from the state of the decoder.

2.1.4 HuggingFace

Huggingface[?] is an opensource known for their contributions for the transformers library, one of the most used libraries for NLP and AI tasks in general. Transformers library provides a wide range of pre-trained models for multiple purposes such as text classification, NER, text generation, translation, etc... It is build on top of the PyTorch and TensorFlow frameworks. Huggingface has played an important role in democratising NLP and making it more accessible, they provide really powerful language models such as BERT, GPT and RoBERTa that can either be used directly, or for transfer learning. They also provide a large range of datasets that can be used for model fine-tuning for various specific tasks.

2.1.5 OpenAI & GPT

2.1.5.1 Generative Pretrained Transformers

GPT models are Language models that have been trained on huge amounts of data such as books, web data and human conversations for the purpose of developping a general understanding of the language.

GPT-1 It all started with GPT the first release by OpenAI[?] in 2018. It had 117 million parameters. It was mainly trained to be able to correctly predict the next word in a sentence. It suffered from the lack of understanding when given a longer context which resulted in incoherent outputs.

GPT-2 In 2019, OpenAI released GPT-2 with 1.5 billion parameter, about 10 times larger than its predecessor. It outperformed the first gen model in the ability of generating coherent text. Due to concerns for misuse, the use of this model was initially very limited. Which will lead OpenAI to perform different types of trainings for their future models.

GPT-3 In their paper “Language Models are Few Shot learners”[?], it was demonstrated how a large model like GPT 3 with a 175 billion can easily learn and adapt to new tasks only using few examples (few-shot learning). Obviously, it also demonstrated better language understanding and impressive performance on multiple NLP tasks such as summarization, question answering and translation

2.2 LangChain

With large language models emerging as a revolutionary technology, Langchain[?], an opensource framework, allows developpers to build applications that were near impossible to make before. Some good examples of those applications are Document Question Answering, Chatbots, Agents.

2.3 Ensemble Learning

Ensemble learning is a Machine Learning technique that combines multiple base models in order to produce a more powerful model that can achieve higher accuracies. By combining the predictions of each base model, we can capture the diverse knowledge and expertise of these models which leads to an improved overall performance. In order to achieve the most optimal results, many aspects need to be considered:

2.3.1 Diversity of Base models

When we talk about ensemble learning, we usually gather multiple models that are considered weak learners. These models have, individually, slightly better performance than random prediction. In order to squeeze the maximum out of this method, the models should be diverse. Diversity ensures that each model brings unique information and makes different errors, reducing the chances of the resulting model being biased or the results being fluctuated by a single model's shortcomings. We can push this further by feeding each model a different subset of our dataset.

2.3.2 Aggregation

Each model in Ensemble learning should predict his own output, then the final result is the aggregation of the multiple outputs. It can be a voting-based method which involves casting votes from each model. The voting can be either HARD, which basically means the majoritarian result is the final result. Or it can be SOFT, which is a weighted vote based on Confidence intervals. The other way to do it is by averaging the outputs. In this method we take the weighted average of the predictions from all the underlying models to get the final prediction.

2.4 Gradient Boosting

Gradient boosting is a type of ensemble learning. The key idea behind it is to iteratively build an ensemble of weak prediction models, where each sub model corrects the errors made by the other models. This iterative process follows the gradient of the loss functions. A very known model for Gradient Boosting is XGBoost:

2.4.1 XGBoost

A Known Gradient boosting machine learning model for his performance and versatility in solving multiple supervised learning tasks. It works as follows:

1. XGBoost starts by initializing a set of weak base models, usually decision trees called a regression tree. Each tree is trying to correct the mistake made by the previous tree. These trees are build sequentially.
2. To define whether the model is performing well, and to guide it in the right direction, a metric or Objective function needs to be defined and optimized during the training process. It is composed of a loss function and a regularization term.
3. The model then computes the gradients of the loss function. It also computes the Hessian matrix to get further information about the curvature of the loss function.

4. The gradients and hessian values are used to determine the best splits when constructing the trees. Each branch is added based on the evaluation of these splits.
5. Regularization penalties are added in order to prevent overfitting and control the complexity of the model to keep it simple. Pruning is also added at the end to further improve the performance and generalization of the model.
6. XGBoost uses early stopping by monitoring the performance of the model on the validation set and stops the learning process when the performance starts to degrade.

Chapter 3

Projects

3.1 Challenge Test Predictions

3.1.1 Presentation of the project

All creams, foundations, and shampoos that become tomorrow's BEST SELLER are the result of a long Research & Development (R&D) process. Before being launched into the market, they undergo microbiology tests, which can make or break their success. If they pass the microbiology tests, it will be a great achievement. If they fail, it will be a nightmare for the formulators who must adjust their formulations to turn their aspirations into reality.

Help has arrived from Cosmetic Factory, a PLM cosmetic software that assists R&D laboratories in speeding up the launch of new cosmetic products. In partnership with the Occitane Group, Ecomundo has developed an Artificial Intelligence (AI)-powered solution to anticipate the outcomes of the Challenge Test (CT). It serves as an intelligent formulation aid for cosmeticians, and was unveiled during the Cosmetic 360 Conference in October 2022. What is a Challenge Test? The Challenge Test is a mandatory pre-market test required by regulations, based on the ISO 11930 method. It involves inoculating a particular concentration of bacteria, such as *Escherichia coli*, *Candida albicans*, *Staphylococcus aureus*, etc. To pass the test, a specific log reduction in the number of microorganisms recovered must be achieved at designated intervals, typically after 2, 7, 14, and 28 days.

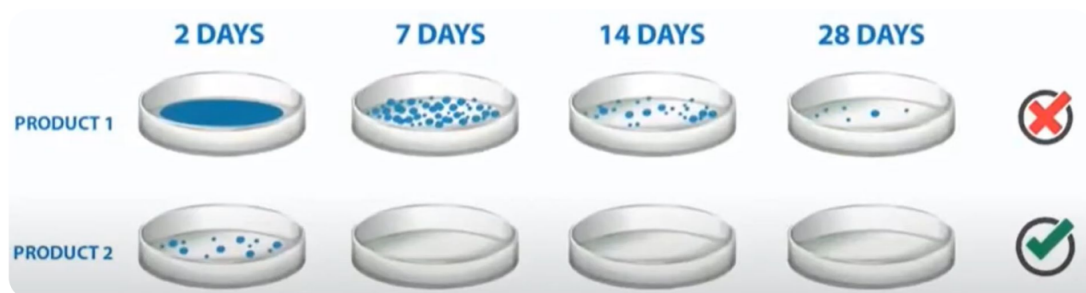


Figure 3.1 – CT

If the specified criteria are not met, as was the case with PRODUCT 1, cosmeticians are required to reformulate and test again until they develop a product that passes the CT, like PRODUCT 2. As a result, one can imagine the laborious nature of the process, as well as the waste of time and resources involved. This is where artificial intelligence comes to the rescue, with its predictive capabilities.

3.1.2 How it is currently done

EcoMundo has developed a hybrid AI solution, which combines an expert system (ES) and machine learning (ML) that predicts the result of the CT, in other words the efficiency of the conservation system. At the moment the solution has been implemented in Cosmetic Factory in the Formulas module, in the Prediction wizard (kyoto server).

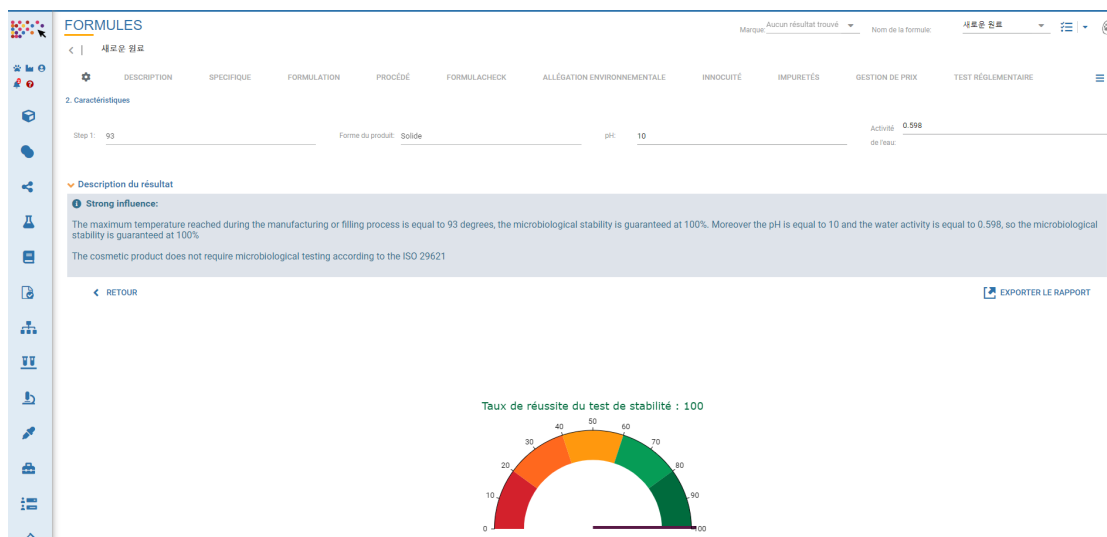


Figure 3.2 – CF interface

To develop the hybrid AI solution we started to study the criteria influencing the risk of microbial contamination. The pH, which measures the acid or basic character of a solution, the water activity that quantifies the free water available to assure growth of microorganisms. Moreover, some raw materials are known to create a hostile environment for the survival of microorganisms like alcohols, inorganic solvents, humectants, inorganic salts, acid and bases. The formulation processes may have an influence on the microbial protection like temperature, incorporation order of ingredients, time of homogenization. And eventually the physical state, if our cosmetic product is a solid, powder, foam etc.. A hybrid system benefits from the reasoning and explanation of the ES, as well as the learning and generalization potential of ML algorithms, which determines an effective and efficient model. This allows users (cosmeticians, formulators, etc..) to understand the prediction, along with the scientific and regulatory reasons behind it. Indeed, the system provides suggestions for improvement, making this solution a useful and

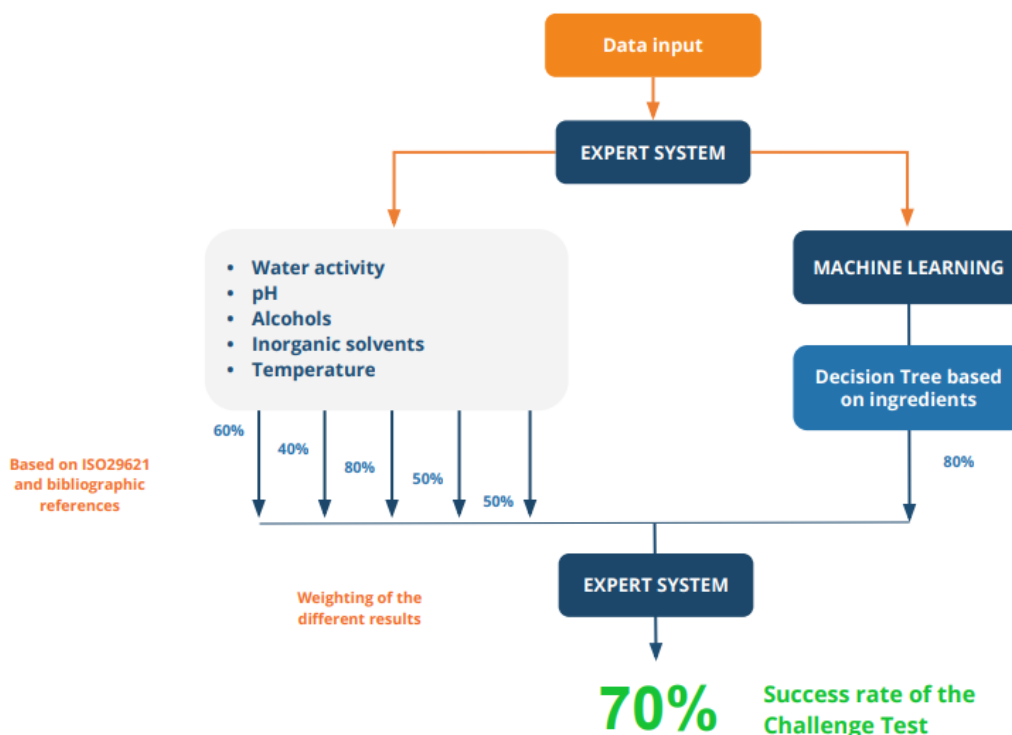


Figure 3.3 – CT flow

reliable formulation support and optimization tool to achieve the success of the challenge test immediately. How is the pipeline structured? The data are feeded to the ES which starts to assign success rate of the CT according to the rules codified in regulation, namely the ISO29621 and based on experimental results published in literature. These rules concern the empiric criteria influencing the risk of contamination based on certain values of pH, water activity, temperature etc. Thereafter, the ES calls the ML to have its success rate. We trained different ML algorithms, but the one that gave the best results is the decision tree applied on the set of ingredients present in the formulas. The result coming from the ML is eventually weighted by the expert system together with the other results, to give finally to the user the success rate of the challenge test.

The ML algorithm chosen is the supervised binary classification, see the decision tree ??, trained on the ensemble of ingredients and their concentration. 3000 formulas furnished by the Group Occitane have been selected and have been divided into 2 sets: a training set which represents 75% and the rest has been used as a testing set. The decision tree at the end gives as answer Yes/No, in other words it is able to say if each formula passes or fails the CT, with a precision of around 80%.

The learning database is composed of formulas, descriptors like pH, water activity and temperature, etc..., which somehow affect the CT results, and of course the CT results. Here, you can find the data conceptual model (DCM) to have a complete vision of the information necessary to train the models.

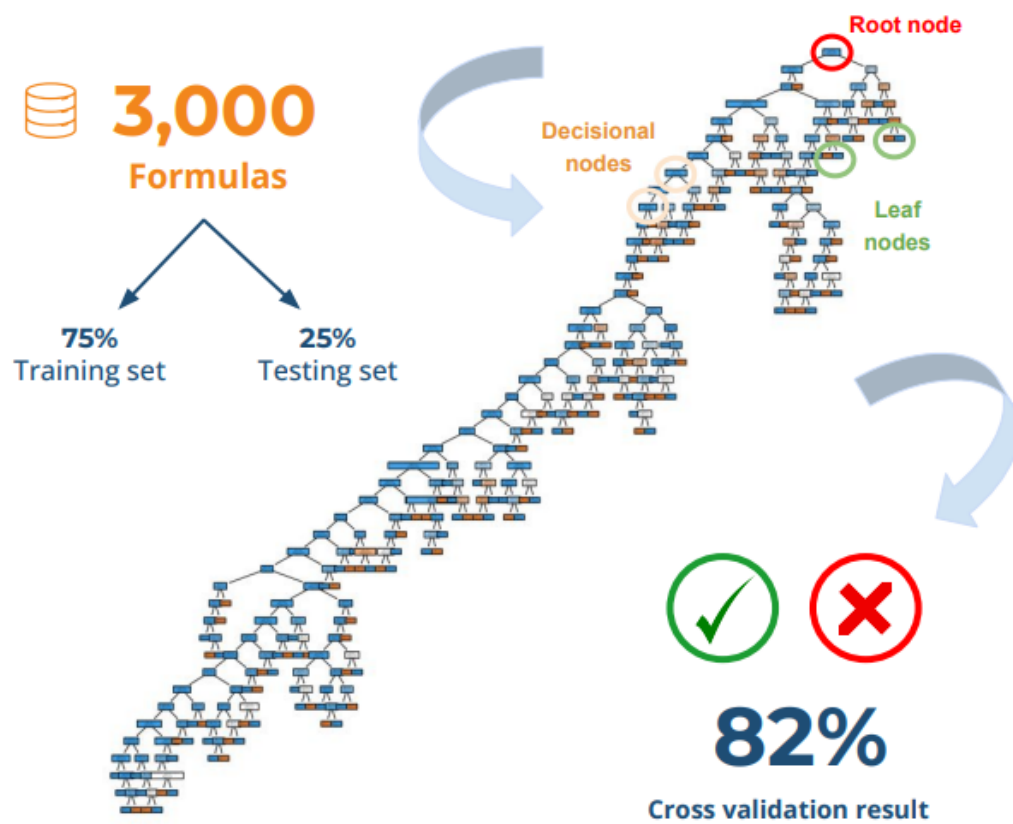


Figure 3.4 – Decision tree

3.1.3 New solution

The new solution is based on ensemble learning. By utilizing multiple models instead of just the decision tree, we will be using XGBoost, Random Forest and a Neural Network (Not implemented yet). In the next subsection, I am presenting the datasets that have been used, the problems with it and how we managed to overcome them.

3.1.3.1 Datasets

These datasets have been provided by L'Occitane ??:

- **ECO_liste des formules avec désignation:** contains list of codes of chemical formulas as well as the type, for example a cream, oil, scrub etc..
- **ECO_formule avec element tech:** Contains the formula code and its corresponding challenge test result.
- **ECO_formule avec liste INCI:** Contains the formula code, ingredients and their corresponding concentration.
- **ECO_formule avec code protocole:** Contains for each formula code, its corresponding protocol code.
- **ECO_code protocole avec liste des codes étapes:** Each protocol of the last table, has many steps. Each step has its own code.
- **ECO_liste des codes étapes avec les conditions:** On each step, some conditions must be respected. Those conditions are in this table like temperature, time with each condition referred to as a code.
- **ECO_formule avec liste MP:** Table that contains for each formula the raw materials in it and their concentrations.

Remarks and problems about the datasets

- CODEMAT and CODEART are the same thing.
- INCI represents one ingredient.
- Raw Material is composed of multiple INCIs (ingredients)
- Total number of Formulas is 7369, though only 5303 have CT results. Out of the 5303, only around 4000 formulas we have their exact compositions with the concentrations.
- Usually, the tests are positives because many hours are spent on making sure the product passes it. This leaves us with a very unbalanced dataset of around 90% of the data have the label "YES", while only 10% did not pass.
- Not all raw materials have the same INCIs, so we have to put all the INCIs in columns and have it at 0 concentration if doesn't exist in the formula. This has left us with a large dataset column wise and it's very sparse (around 80 percent of the values are zeros).

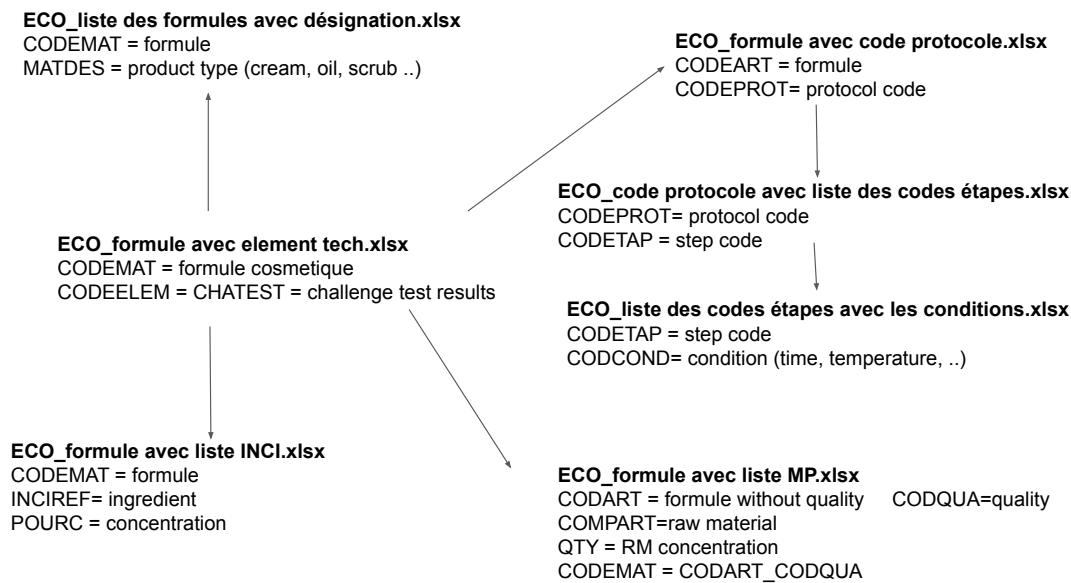


Figure 3.5 – Datasets L’Occitane

To tackle these problems, first we needed to do a stratified split on the dataset in order to well train it. Then imperatively use PCA in order to reduce the size of the dataset. (code is not included in the report, will be presented live).

3.1.4 ML Pipeline and Deployment Architecture

Following the figure ??, this is how the ML pipeline is structured:

1. We have implemented a robust data collection mechanism to gather the required data from the EcoMundo database using SQL scripts. The collected data is then transformed into a CSV file for further processing.
2. For now, we have used a Google Colab notebook, where we perform extensive preprocessing on the collected data to ensure it is in a suitable format for ML model training. Using the pandas library, we create a structured dataframe. We then employ scikit-learn and TensorFlow libraries to train various ML models. Through optimization and fine-tuning techniques, we enhance the model’s performance.
3. To integrate the ML model into the existing Cosmetic Factory software, we have designed and developed an AI application using the Django framework. This application is called when there is no response from the Rule Engine. Through a REST API, a Java controller in the back-end is called, allowing communication between the ML model and the software.
4. We have implemented a mechanism for real-time inference, enabling the ML model to make predictions in real-time. The ML model’s predictions are integrated with the existing software’s logic. This process involves

making API calls to retrieve answers, which are then sent to the Java controller and displayed in the application's front-end.

5. We have set up a manual periodic fine-tuning process to retrain the ML model using new data from the EcoMundo database. By incorporating user feedback and leveraging the latest data, we continuously improve the model's accuracy and effectiveness.

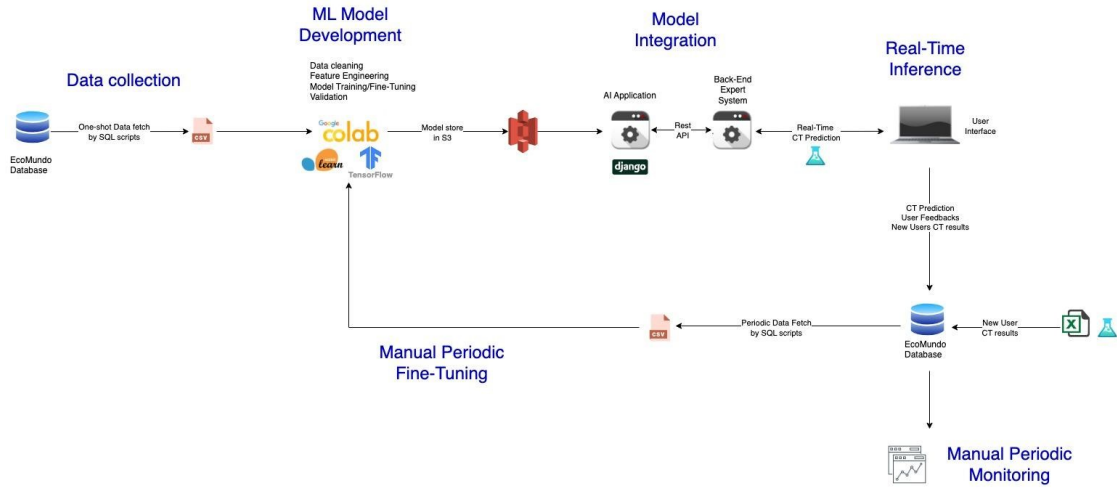


Figure 3.6 – ML Pipeline

3.1.5 Results and Comments

3.1.5.1 Metrics

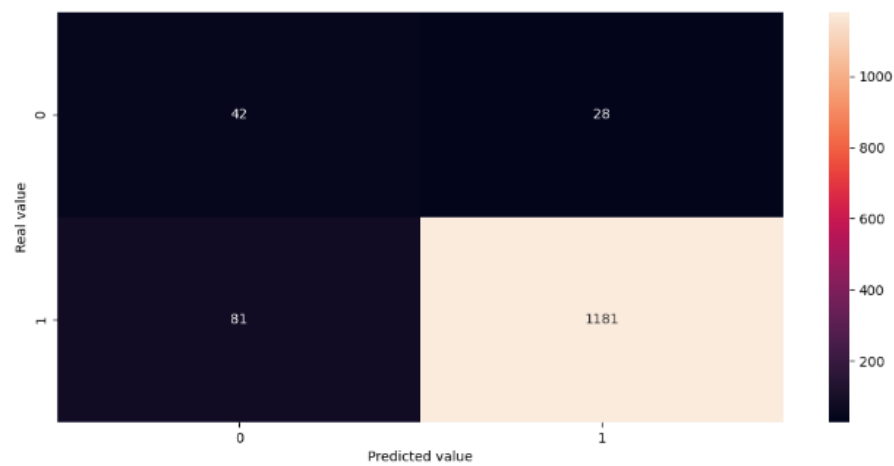
Because we are working on a binary classification, precision alone is not a good metric for how performant the model is. This metric only computes how many times a model made a correct prediction across the entire dataset. Recall on the other hand measures how many of the positive class samples present in the dataset were correctly identified by the model. F1-score is the best for this use case, since it's compatible with unbalanced datasets and it combines both recall and precision.

$$F_1 = 2 * \frac{precision * recall}{precision + recall}$$

Another Metric that we have used is the ROC AUC score. It reflects on how efficient the model is. The higher the Area Under the Curve, the better model's performance at distinguishing between the two classes.

The expert actually wanted less false negatives and did no care about the other metrics. If we gave as a result that a formula will pass the challenge, but when its conducted it does not pass, it's not as big of a problem as the other way around: We say it is not going to pass the test but it actually does.

3.1.5.2 Results



```

accuracy score: 0.9181681681682 %
auc score: 0.8216022110593315

```

	precision	recall	f1-score	support
0	0.34	0.60	0.44	70
1	0.98	0.94	0.96	1262
accuracy			0.92	1332
macro avg	0.66	0.77	0.70	1332
weighted avg	0.94	0.92	0.93	1332

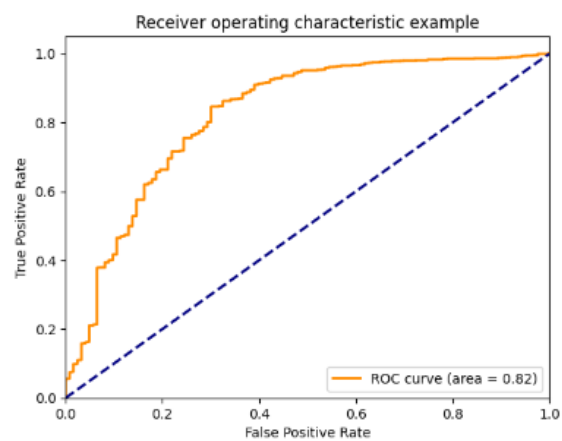


Figure 3.7 – XGBoost Confusion Matrix, AUC

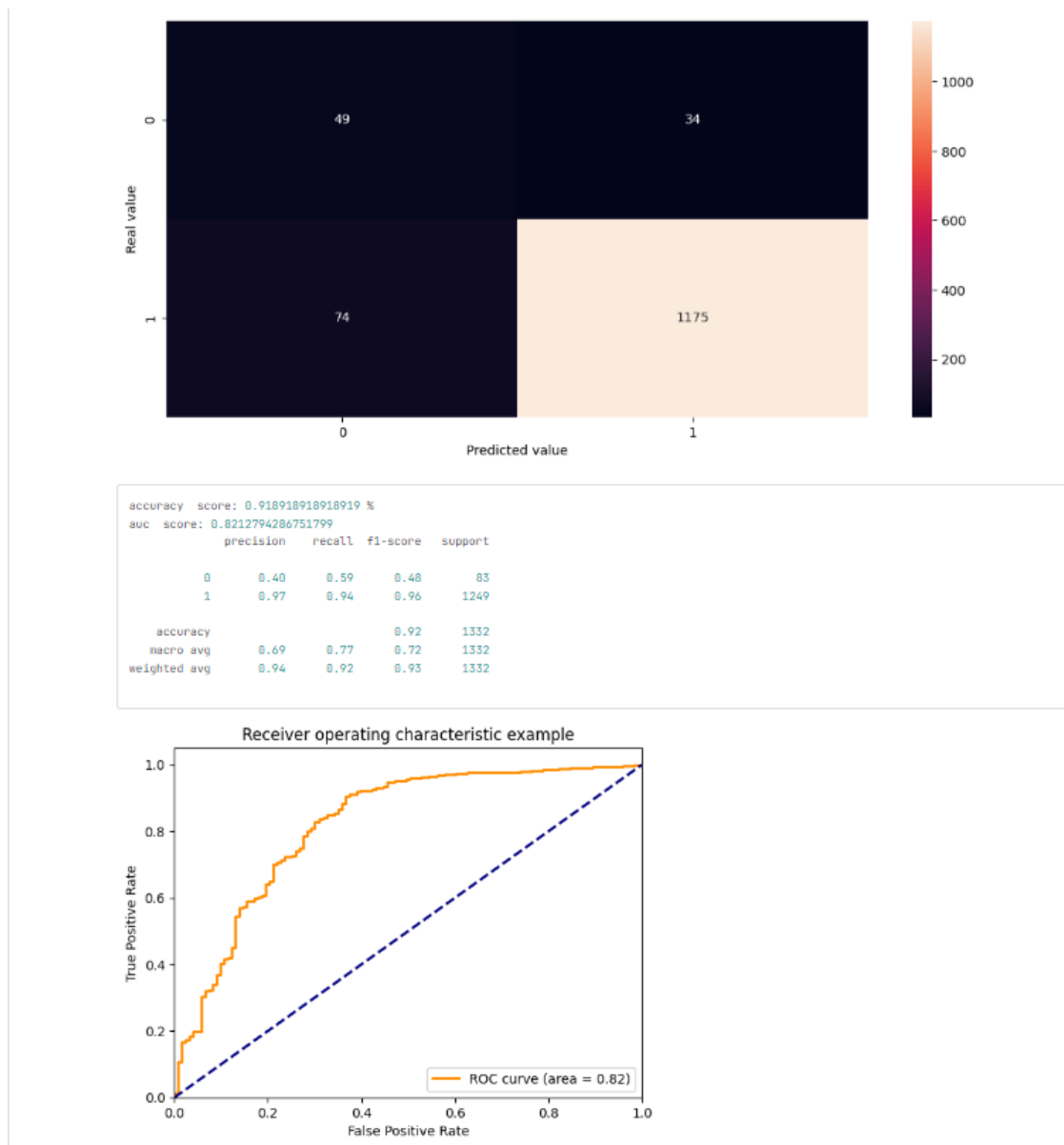


Figure 3.8 – Random Forest Confusion Matrix, AUC

3.1.5.3 Comments

The result that we got on the inference of these two models have been enough to support the Expert system in its prediction. At the end of the day, I suggested that we do not take 50% as the threshold of classification. This means if for example a product had a 60% for example of passing the challenge test, we would show the percentage and our expert suggestion that effecting the challenge test for this product will probably be a loss of time and money in case of failure.

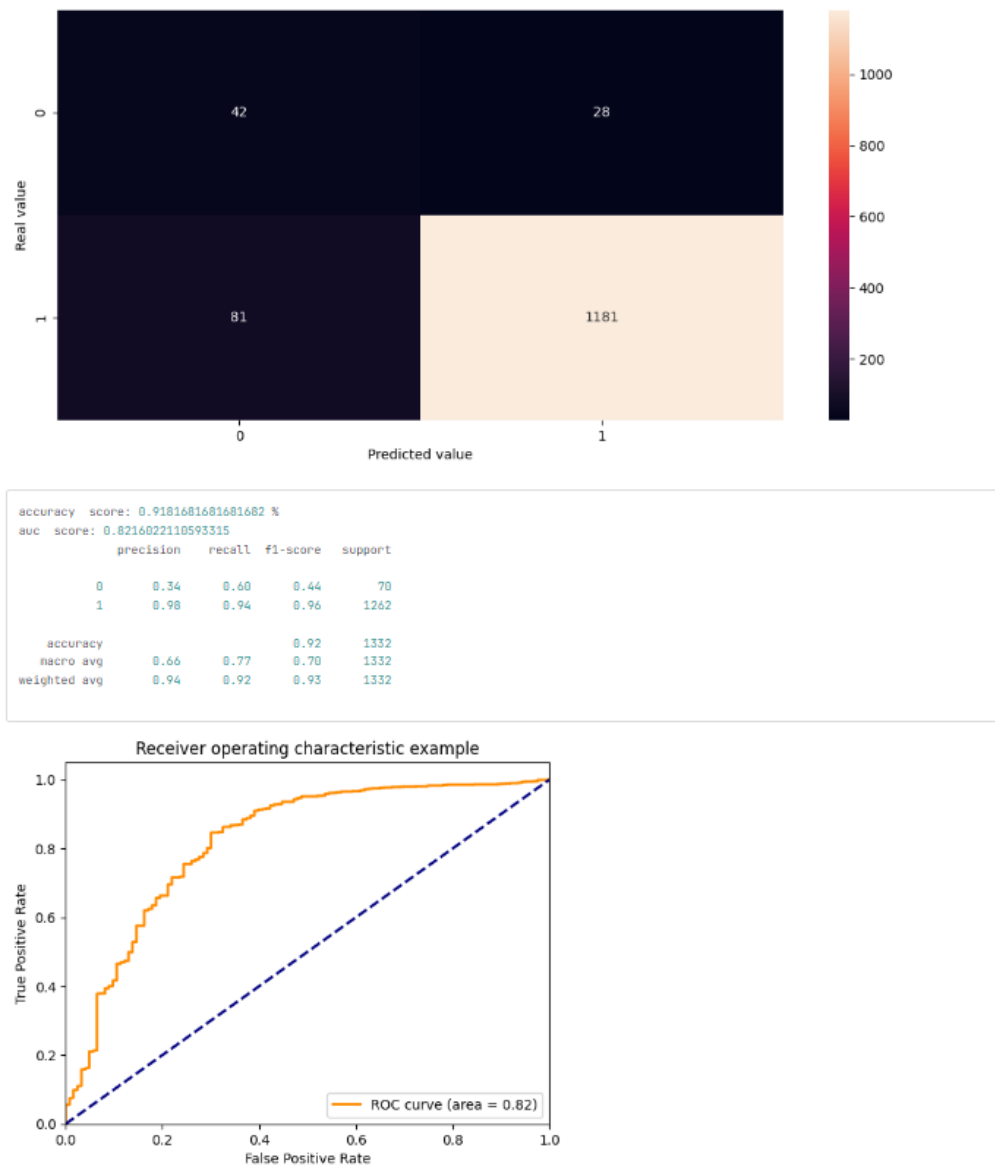


Figure 3.9 – XGBoost Confusion Matrix, AUC

3.2 SDS Reader

3.2.1 Presentation of the project

Currently called PDF Reader, is an application made by Ecomundo specifically for Safety Data Sheets:

3.2.1.1 What is an SDS?

Safety Data Sheet, also known as Material Safety Data Sheet (MSDS), is a very important document that provides informations about the hazards and safe handling of a specific substance/mixture. Its main purpose is to ensure

the safety of individuals who may use or come in contact with the substance in any settings. It is composed of sixteen sections:

- **Identification:** Identification of the substance/mixture on the SDS as well as the recommended uses. It contains also the contact informations for the suppliers/manufacturers
- **Hazard Identification:** This section identifies the hazards of the substance/mixture presented in the SDS along with their appropriate warning informations
- **Composition/Information on Ingredients:** This section identifies the substance(s) contained in the product, their concentration and their hazard classification.
- **First-Aid Measures:** Descriptions of the initial care that should be given by untrained responders to an individual who has been in contact with the chemical.
- **Firefighting Measures:** Recommendations for fighting the fire caused by the chemical.
- **Accidental Release Measures:** This section has recommendations on the appropriate responses to spills, leaks or releases including containment and cleanup practices to minimize or ideally prevent exposure to the people and the environment.
- **Handling and Storage:** Guidance on the best and safe practices of handling and storing the product.
- **Exposure Controls/ Personal Protection:** In this section, the exposure limits, engineering controls and personal protective measures are indicated.
- **Physical and Chemical Properties:** This section identifies the physical and chemical properties of the substance/mixture
- **Stability and Reactivity:** This section provides information about the reactivity hazards of the chemical and its stability information.
- **Toxicological Informations:** Informations about the toxicological and health effects.
- **Ecological Information:** This section provides information to evaluate the environmental impact of the substance(s).
- **Disposal Considerations:** Guidance on proper disposal practices, recycling or reclamation of the substance(s) or its container and safe handling practices.
- **Transport Information:** Guidance on classification information for shipping and transporting of hazardous substance(s) by road, air, rail, or sea.
- **Regulatory Information:** Safety, health and environmental regulations specific for the substance/mixture that is not indicated anywhere else on the SDS.
- **Other Information:** Indications about the preparation and revision date of the SDS along with other useful information such as the changes that have been made compared to the last version.

3.2.2 How it is currently done

3.2.2.1 Get sections

The old code is a static code that mainly starts by dividing the pdf into paragraphs. then go through each paragraph and detect where the sections are by comparing the words to the words that define sections in the SDSFactory database. For example you can have "SECTION" as the word splitting the document into sections, might also be "RUBRIQUE" if it's in French. It uses all possible words that are available in the database in the language of the SDS.

3.2.2.2 Get Key-Value pairs

Using Regular Expressions, the code then goes through each section and finds all the key value pairs that are mentioned in the PDF file. This is already problematic since there are inconsistencies of how a key value pair is shown in the file: It could be in the form of Key:Value, sometimes it's Key n Value.

3.2.2.3 Match with Ecomundo Template

Using the same static method of looking into the database, the code then goes through all the key value pairs and matches them with the Ecomundo Template of Keys.

3.2.3 Problems with the old way

As it is very obvious, the static way of searching through the database for keywords, and expecting to have the exact same match is far from optimal. If we have an SDS with a different language then we have to recreate a table in the database for that exact same language, then fill it with all possible words for each key. For example the key "Product Name" can be in the pdf as "Product identifier" or just "Name", if we don't have these keys in the database, it will assume this data does not exist in the pdf. We notice as well the workload of refreshing and updating the database frequently in order to keep it updated.

3.2.4 New solution

3.2.4.1 Usage of Large Language Models

The usage of large language models was first proposed as it will allow us to read the pdf and understand it then extract data from it. This method as demonstrated first by using ChatGPT and giving him texts in different languages from an SDS and providing him the keys to extract. Two major problems have arisen from the proposition of using this method:

Security Sending PDF files of clients to OpenAI servers in North America for processing is not a straightforward procedure. The Technical directors were worried about data privacy of the clients even if SDS are not considered confidential in most cases. But as we will be using GPT models using the OpenAI api, and as a company, I suggested we contact sales and request to not store our sent data after the processing is done. It is a right that anyone can ask for when purchasing the api key[?].

Cost At the time of the first meeting 13th March 2023, the pricing for gpt-3.5-turbo model was 0.002 USD/1000 Tokens. The commercial team were not convinced of how cheap it is until I presented a proof of concept later on.

3.2.4.2 Open-Source Large Language Models

To tackle these two problems, I proposed to postpone the GPT api purchase while I dig deep into how we can use an opensource model. I started by looking into the models that are Open Source + Available for commercial use:

BERT and its derivatives The BERT model [?] (Bidirectional Encoder Representations from Transformers) was introduced in 2018 by researchers at google. It achieved state-of-the-art performance on many NLP benchmarks. In my proposition to use open source models, BERT models came in as top results. BERT model was optimized when RoBERTa [?] (Robustly optimized BERT) was introduced in 2019 which was optimized even more with the introduction of DeBERTa [?] (Decoding-enhanced BERT with disentangled Attention).

I started initially by using these models for question answering. The PDF file would be converted into a raw text file, then fed to the model as context. Then I gave it the keys that I wanted to extract. DeBERTa Model was the best obviously, but still lacked in many areas:

Bad extraction The model was very inconsistent with the extractions, some keys would be perfectly extracted while other were not. The model also does not quite understand the structure of the page only from the raw text given to it as context. Finetuning is always an option with these models, for the lack of time that I had with them on-site, and the deadline that we had for the end of June, we have proceeded to the usage of other solutions.

3.2.4.3 GPT

OpenAI has made the model gpt-3.5-turbo available from their api for as cheap as 0.0015 USD/1K tokens (June 2023). To demonstrate the power of the model and how cheap it can be, I did a demo doing extraction of all

key value pairs of an SDS page by page. It costs around 0.01 Euros per pdf of 13 pages. This has captured the attention of Christian FRENEUIL, the Software and Cloud services Sales Director, and pushed this project.

First Version of the stable code: Non-Hybrid This code works as follows:

1. Extract all key value pairs from each page. Keep a record of what sections are in that exact page, and save the latest one. For example if a page has Section 1 and Section 2, we save them both in an array, then we save the fact that section 2 was the latest.
2. When we move to the next page, we check whether the page starts directly with a section, then we assign the key values of that section to the corresponding key, if not we assume it's the Section 2 continued.
3. Group by Sections then send it to another controller in the application that will then match the key value pairs from each section into the keys that we have.

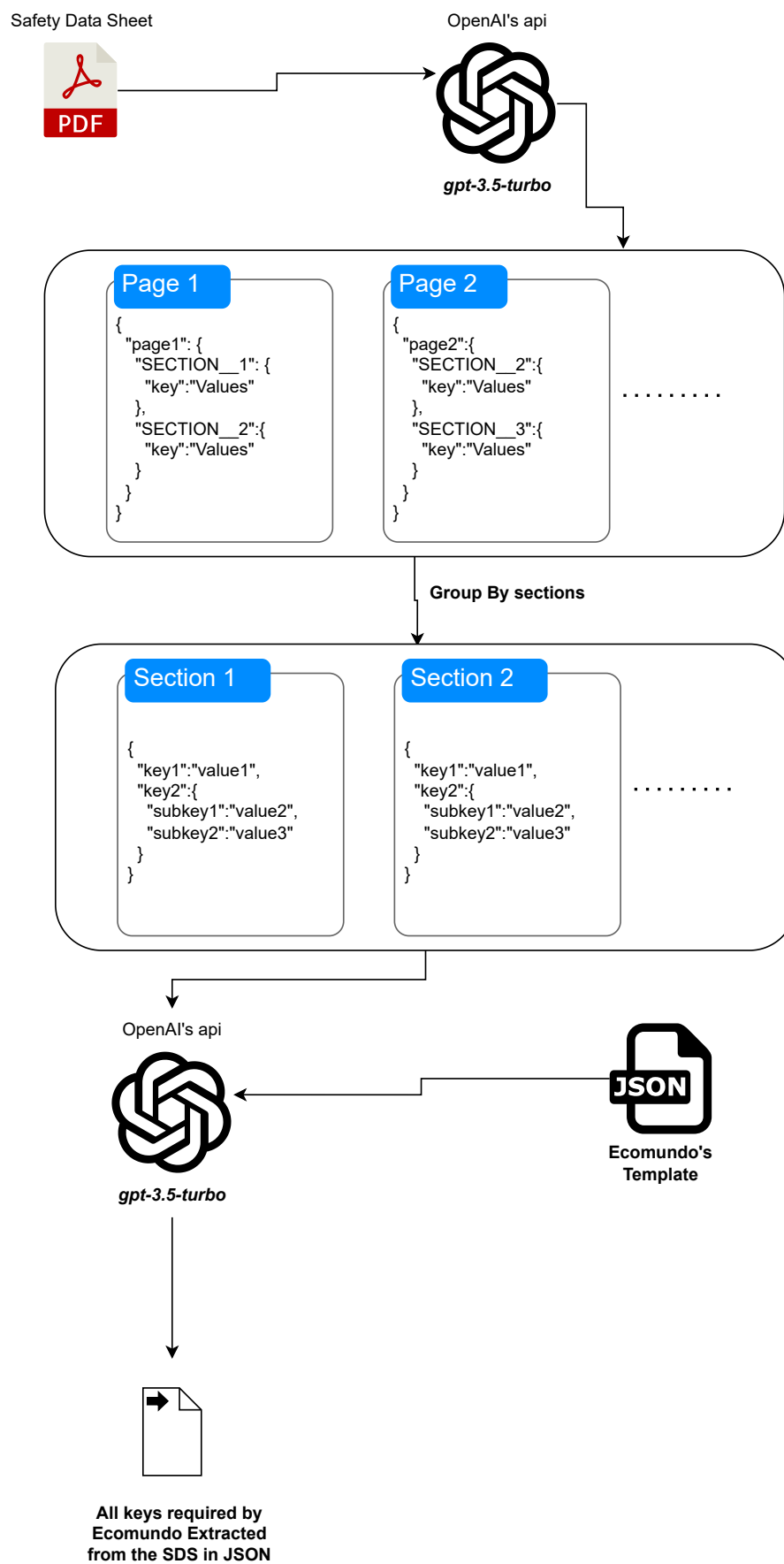


Figure 3.10 – Non-Hybrid
Academic Year 2022 - 2023

Hybrid Version of the code As it is obvious in ??, we are using OpenAI's api twice. The first extraction is taking an overhead task of detecting sections, that in some cases fail. To overcome this problem, we thought about using the existing PDFReader controller that splits the SDS into sections, and then use them directly for extraction and matching. This will give us Two benefits:

1. **Parallel extraction:** We will be able to parallelize the extraction for each section, and the extraction by Ecomundo's template for each section. Which means the complexity of this extraction will be the complexity of the longest Section.
2. **Better Extraction:** Since we are focusing on only one task, the gpt model will work better with a one-goal instruction rather than multiple ones.

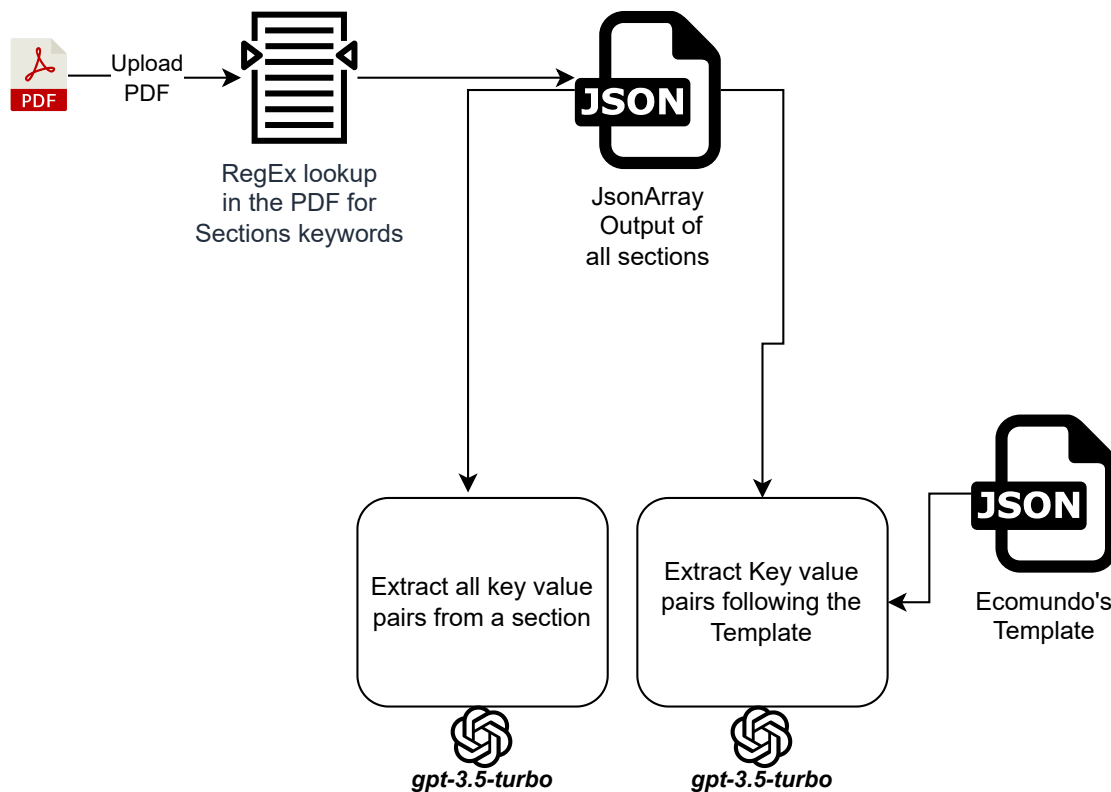


Figure 3.11 – Hybrid

Even More improvements To tackle problems relating to either: Size of the context (in our case the raw pdf text) and/or the quality of section extraction, I proposed a further architecture improvement. ??

1. The pdf is loaded into the SDSReader interface, we first extract the text, if the text is empty, this means it's not a digital PDF. We then use PyTesseract OCR to extract the text.
2. Check for the quality of section extraction. If the length of the sections' list is not 16, we assume we did not correctly extract and we use the

previous stable code. If it's till not 16 sections, we move to the langchain solution for the entire pdf proposed in ??.

3. Assuming we had 16 sections, before the extraction, we need to check for the context limit of the prompt+the raw text. If we are in the context window of gpt-3.5-turbo, which is 4097 tokens, we are good. If not, we check if it's less than 16K tokens, then we use gpt-3.5-turbo-16k, which costs about 0.003 for input tokens and 0.004 for output tokens. If we are still outside this range, then we use LangChain solution but for only that exact section.

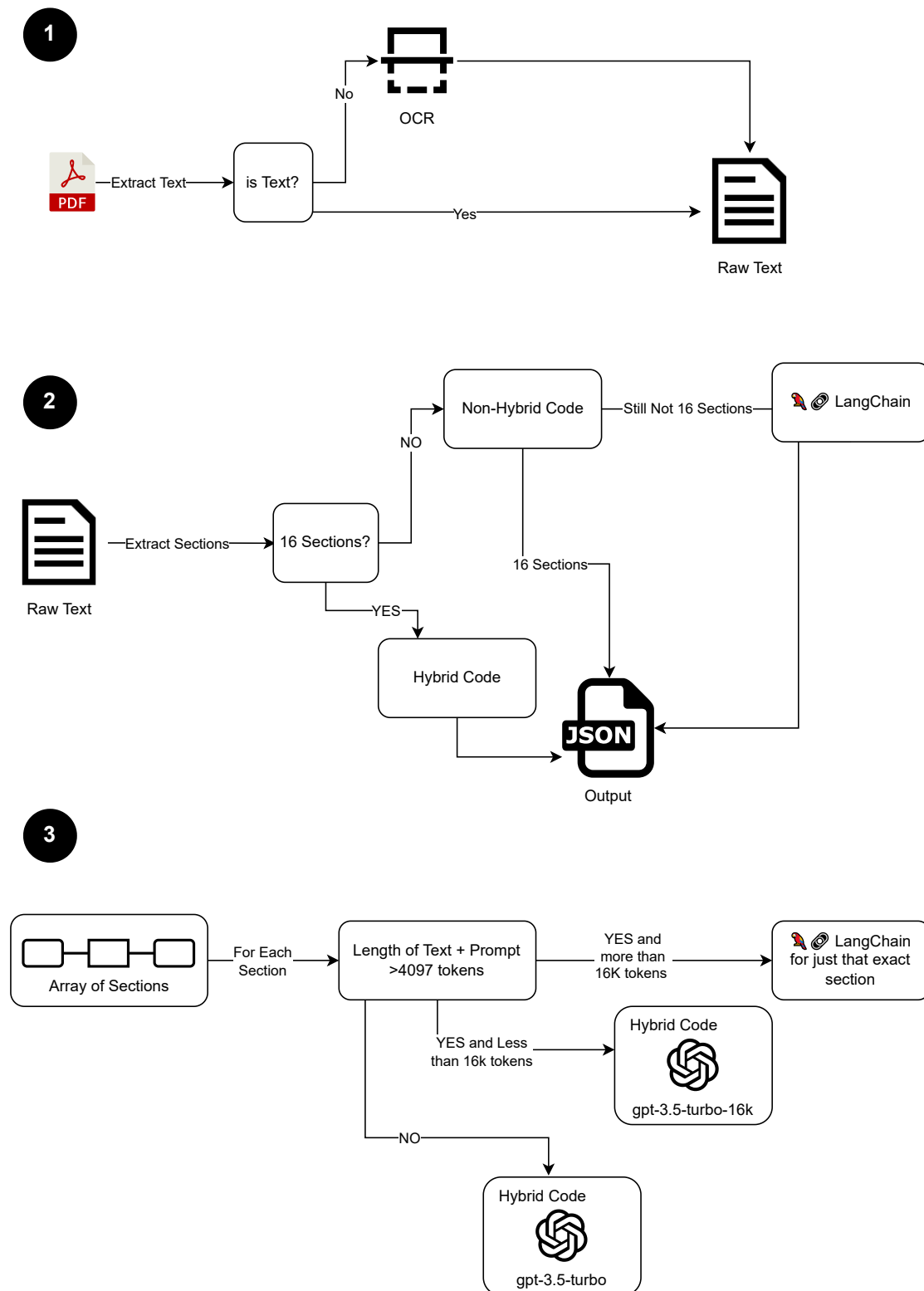


Figure 3.12 – Hybrid++

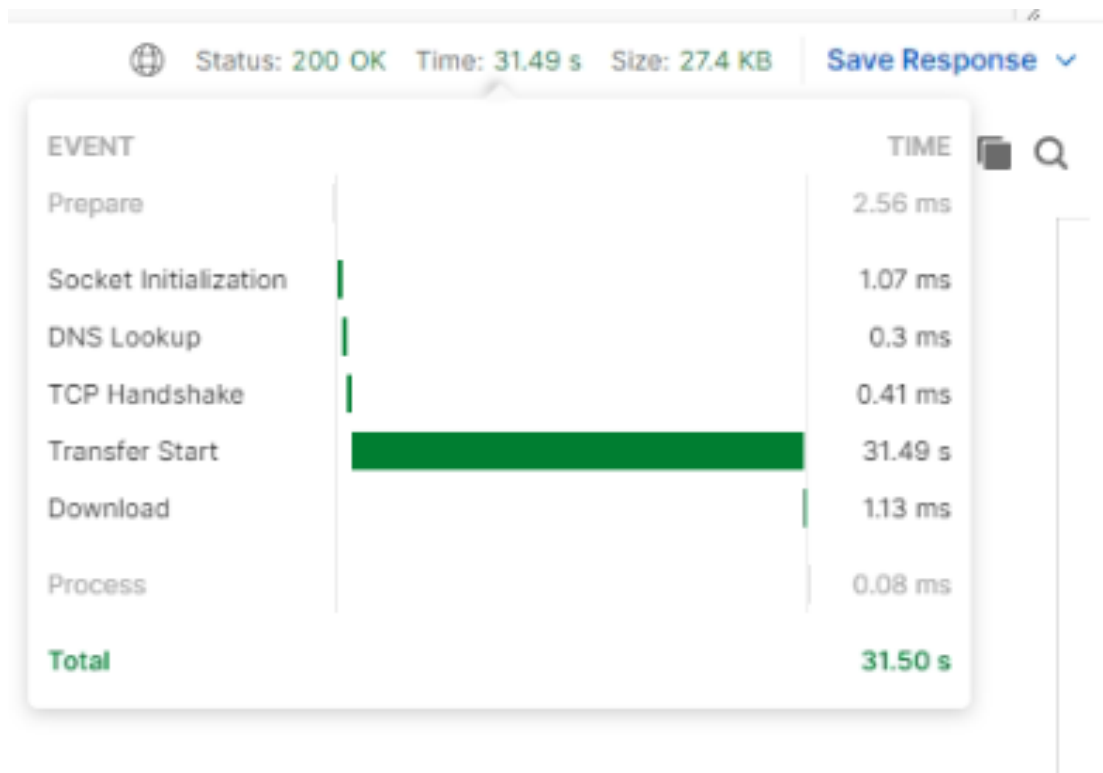


Figure 3.15 – Extraction Time for new SDSReader

3.3 ChatBot: EcoMundo Smart Assistant

3.3.1 Presentation of the project

With the release of ChatGPT, the chatbot paradigm has shifted from simple Question Answering models to a human-to-human interaction. In Ecomundo, the idea of having a chatbot was needed to answer clients' frequently asked questions as well as special cases. The ideal solution would be a chatbot integrated in all of Ecomundo's Applications (Starting first as a beta version with Cosmetic Factory).

With a chatbot powered by gpt-3.5-turbo (or whatever latest and high quality per price range model is available), this project is very doable.

3.3.2 Theoretical solution

The problem with using a gpt model directly, is that it has zero knowledge about our software (Obviously it was never intended to be used directly), has little to zero knowledge about the updated regulations since its training database dates to april 2021. The first solution that comes to mind is to fine tune it with our database of questions already answered by the commercial team as well as the latest regulations and documentation about our software. But this will be a financial hit since the model fine-tuned costs 0.12 USD/1K

tokens (6 times more expensive than normal DAVINCI model) + 0.0300 / 1K tokens for training it. We need another solution:

3.3.2.1 Langchain: Context Injection

Langchain as I briefly described in ?? is an opensource framework that allows the users to create agents, chatbots and question documents using Large Language Models. It mainly works using a method called **Context Injection**. This method involves using vectorstores in order to calculate similarity searches between the embedding of the user's question and our context documents. If there is already a chat history with the chatbot, we will create a standalone question that reformulate the questions taking into consideration that history.

The context documents will be splitted into chunks, so the search will actually be between the query and the chunks. The figure ?? explains exactly how this method works:

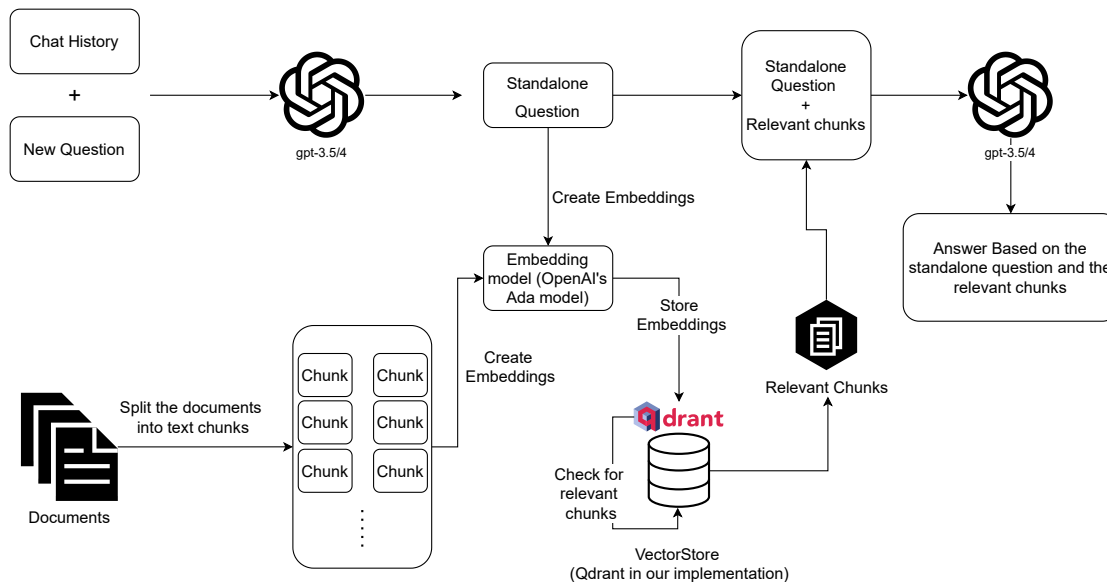


Figure 3.16 – Context Injection using GPT Models

1. We start by taking the client's question and combining it in a comprehensive way with the chat history if it exists, then we generate a standalone question using GPT model. We create using an embedding model like OpenAI's ADA for the standalone question.
2. We then take our context documents and split them into text chunks. We also embedd these chunks using the same model. **This step will be done only once unless we add new documents in the future.**
3. We compute using the cosine similarity (or any other similarity metric) to extract the top chunks that are relevant to our question. **This step is the weakest link in this architecture since it's dependent on how good the similarity metric is.**

4. We combine the standalone Question and the relevant chunks and we send them as a request to GPT model again. This step can be done with Langchain in four ways:
 - (a) **Stuffing:** Takes all the context and puts it in one request with the question.
 - (b) **Map Reduce:** Sends multiple requests in parallel, each one with a chunk of text. At the end it combines all the answers in one final answer.
 - (c) **Refine:** Sends multiple requests in sequences, each one with a chunk of text. After having an answer from one request, it is refined using the next context chunk, if no improvements are possible then the previous answer is preserved.
5. We output the final Answer to the user.

3.3.2.2 Future work

This project was only introduced as a concept, we managed to make a proof of concept when we used it in PDFReader in the case of a very long section or when a document that we was not splitted correctly into sections. We still need to test it again with its main purpose which is a chatbot, figure out how to integrate it into our softwares and obviously how impactful it will be for the clients.

Bibliography

- [1] Tom B. Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agarwal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, Daniel M. Ziegler, Jeffrey Wu, Clemens Winter, Christopher Hesse, Mark Chen, Eric Sigler, Mateusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCandlish, Alec Radford, Ilya Sutskever, and Dario Amodei. Language models are few-shot learners, 2020.
- [2] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding, 2019.
- [3] Ecomundo. Conformité internationale - Services & Logiciels | Eco-Mundo. <https://www.ecomundo.eu>, 2023. Accessed on June 5, 2023.
- [4] Pengcheng He, Xiaodong Liu, Jianfeng Gao, and Weizhu Chen. Deberta: Decoding-enhanced bert with disentangled attention, 2021.
- [5] HuggingFace. The AI community building the future. <https://huggingface.co/>, 2023.
- [6] LangChain. Building applications with LLMs through composability. <https://github.com/hwchase17/langchain>, 2023.
- [7] Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. Roberta: A robustly optimized bert pretraining approach, 2019.
- [8] Tomas Mikolov, Kai Chen, Greg Corrado, and Jeffrey Dean. Efficient estimation of word representations in vector space, 2013.
- [9] OpenAI. OpenAI. <https://openai.com/>, 2023.
- [10] OpenAI. OpenAI Usage Policy. <https://openai.com/policies/api-data-usage-policies>, 2023.
- [11] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017.

Appendices

Appendix A

Appendix

```
1  include:
2    - template: Jobs/SAST.gitlab-ci.yml
3    - template: Jobs/Dependency-Scanning.gitlab-ci.yml
4    - template: Jobs/Secret-Detection.gitlab-ci.yml
5    - template: Docker.gitlab-ci.yml
6
7  stages:
8    - lint
9    - test
10   - container-build
11
12  .python-req:
13    image: python:3.9
14    before_script:
15      - pip3 install pyflakes
16    script:
17      - pip install -r requirements.txt
18
19  lint-python:
20    extends: .python-req
21    stage: lint
22    allow_failure: true
23    script:
24      - pyflakes .
25
26  sast:
27    stage: test
28
29  docker-build:
30    stage: container-build
31    image: docker.io/ecomundoit/worker:1.22
32    before_script:
33      - echo "${DOCKER_IO_PASSWORD}" | podman login --username "${DOCKER_IO_USER}" --password-stdin docker.io
34    script:
35      - "[ -f ./build.sh ] && ./build.sh"
36      - IMAGE_FULL_PATH="docker.io/ecomundoit/${CI_PROJECT_NAME}:${echo "${CI_COMMIT_REF_NAME}" | sed -E 's/^master|main$/latest/g')"
```

Figure A.1 – Python CI pipeline



FINECOAT

Material Safety Data Sheet

PT21-S

 Page 1/6
 Revision Date: July/29/2022

1. PRODUCT / COMPANY IDENTIFICATION	
Product Name	: PT21-S
Chemical Identification	: Heat curable coating material
Manufacturer's Name	: Finecoat Co., Ltd.
Address	: 340-1, Banwol-Dong, Hwaseong-Si. Gyeong-gi-Do, 18384, KOREA
Phone No.	: 82-31-225-6201
Fax No.	: 82-31-225-6207
Emergency Phone No.	: 82-31-225-6201

2. HAZARDS IDENTIFICATION	
A. Hazards. Dangerousness identification	
Flammable Liquid : Division 2	
Acute toxicity (Oral) : Division 3	
Acute toxicity (Skin) : Division 3	
Heavy Eye Damage / Eye irritation : Division 1	
Specific Target Organ Toxicity (Once Exposure) : Division 1	
Specific Target Organ Toxicity (Exposion repeatedly) : Division 1	
B. Warning Signs items which include Prophylactic measures	
Pictorial Symbol	
Signal Words	Risk
Harmful / Risk phrases	H225 High Flammability Liquid and Steam H301 Harmful if swallowed H311 Harmful to contact skin H318 Causing eye damage
Prevention action phrase	
Prevention	P210 keep away from heat, sparks, flames and high Fever-No smoking P233 Seal the container tightly . P240 Join or ground containers and receptacles.

RESEARCH & DEVELOPMENT DEPARTMENT / FINECOAT CO., LTD.

Figure A.2 – Demo Chapter 2



FINECOAT

Material Safety Data Sheet

PT21-S

Page 2/6
Revision Date: July/29/2022

Response	<p>P241 Use explosion-proof, electrical ventilation lighting Equipment</p> <p>P242 Use only non-sparkling tools</p> <p>P243 Take precautionary measures against static discharge</p> <p>P260 Do not inhale dust, gas, mist, or vapor</p> <p>P264 Wash the handling area thoroughly after handling</p> <p>P270 Do not eat, drink or smoke when using this product.</p> <p>P280 Wear protective gloves, protective clothing, safety glasses, and facial protection</p> <p>P301+P310 If swallowed, consult a doctor immediately</p> <p>P301+P330+331 Wash your mouth if you swallow it swallowed. Don't try to throw up</p> <p>P302+P352 Wash with plenty of water if it gets on your skin.</p> <p>P303+P361+P353 If it gets on your skin, take off your contaminated clothing and take a shower.</p> <p>P304+P340 When inhaled, move to fresh air and rest in easy breathing position.</p> <p>P305+P351+338 Carefully wash with water for a few minutes if it gets on your eyes. If possible, remove contact lenses and continue washing</p> <p>P308+P313 If you are concerned about exposure or exposure, consult a medical institution (doctor).</p> <p>P310 Consult a doctor immediately</p> <p>P312 If you feel uncomfortable, consult a medical institution (doctor).</p> <p>P314 Measures get medical advices If you feel Uncomfortable.</p> <p>P330 Rinse the mouth</p> <p>P361+364 Remove all contaminated clothing immediately and clean before using again.</p>
Storage	<p>P363 Clean contaminated clothing before using it again</p> <p>P403+P235 keep container tightly closed and store in well-Ventilate place.</p>

RESEARCH & DEVELOPMENT DEPARTMENT / FINECOAT CO., LTD.

Figure A.3 – Demo Chapter 2


FINECOAT

Material Safety Data Sheet

PT21-S

 Page 3/6
 Revision Date: July/29/2022

Disposal	P405 Store in a lock storage place P501(As specified in the relevant laws) Dispose of the contents of the container.	
C. Hazardous which is not included in other dangerous risks.		
Health	1	
Fire	3	
Reactivity	0	
3. COMPOSITION/INFORMATION ON INGREDIENTS		
Components	CAS No.	Content
Polyester resin	65072-11-9	2-4 wt%
Silicone Dioxide	7631-86-9	2-4 wt%
De-Ionized water	7732-18-5	20-30 wt%
Methyl Alcohol	67-56-1	50-65%
4. FIRST AID MEASURES		
Inhalation	: Remove to fresh air. Give artificial respiration if not breathing.	
Skin Contact	: Wash skin with soap, rinse with water, seek medical attention.	
Eye Contact	: Immediately flush eyes with water for at least 15 minutes, then obtain medical attention.	
Ingestion	: Do not induce vomiting, if vomiting should occur spontaneously keep airway clear, seek medical attention.	
Others	: Never give anything by mouth to an unconscious person. Discard contaminated clothing and shoes immediately.	
5. FIRE FIGHTING MEASURES		
Extinguishing Media	: Carbon dioxide, dry chemical media, appropriate foam	
Explosion Hazards	: Keep container cool by spraying with water if exposed to fire. Product may polymerize at high temperature. Polymerization is a highly exothermic reaction and may produce sufficient heat to cause thermal decomposition and/or rupture of container. Vapor may travel considerable distance to source of ignition and flash back	
Special Equipment	: Self-contained breathing apparatus and protective clothing should be provided to fire fighters in building or confined area where this product is stored	
6. ACCIDENTAL RELEASE MEASURES		

RESEARCH & DEVELOPMENT DEPARTMENT / FINECOAT CO., LTD.

Figure A.4 – Demo Chapter 2

Abstract

This report presents the findings and outcomes of three projects that utilized artificial intelligence (AI) to enhance operations in the chemical regulations industry.

The first project aimed to develop an AI-powered solution for predicting the outcomes of Challenge Tests, which evaluate the effectiveness of cosmetic products in inhibiting the growth of microorganisms. By analyzing the formulation of cosmetic products using machine learning algorithms, the solution provided accurate predictions of Challenge Test outcomes. This optimization allowed formulators to improve their formulations and increase the likelihood of passing the tests, thereby reducing the time and resources needed for product development. This project was conducted in collaboration with the L'Occitane Group and integrated into the Cosmetic Factory software, a Product Lifecycle Management (PLM) solution.

The second project focused on developing an AI solution for reading Safety Data Sheets (SDS). The existing solution used a static code to search for keywords in PDFs and match them with a database. However, this approach had limitations in handling different languages and variations in key-value pairs. The new solution proposed the use of large language models and context injection to improve extraction accuracy and efficiency. This enhanced the ability to extract key information from SDS, improving safety and compliance in the cosmetics industry.

The third project aimed to develop a chatbot powered by a large language model to provide support and answer frequently asked questions. However, the cost of fine-tuning the model with the company's database was prohibitive. As an alternative, the Langchain framework was proposed, which utilized context injection to provide relevant answers based on the user's question and available context documents. This chatbot solution improved customer support and efficiency in addressing client inquiries.