The problem of chemical formulation of a compound (Compounding) regards the structural modification actions that must be applied to a chemical compound object, in order to obtain a pre-defined set of desired features and performances of the compound.

A chemical compound object is represented by a recipe (a finite set of ingredients).

Given a race within a championship in a circuit with its geometrical profile and road ground, in some place in the world, in a certain season with some weather conditions, with a specific car with its characteristics, and a specific car driver; given information about the previous race in the same circuit at the previous championship, and given the previously used recipe of the rubber compound composing the thread batch.

What will be the right chemical formulation to be implemented into the rubber compound to win this race?
**Case Based Reasoning**

**Cogntive Perspective**

“Case Based Reasoning is a psychological theory of human cognition. It addresses issues in memory, learning, planning and problem solving.” (S. Slade, 1991)

Case Based Reasoning is the process of solving new problems on the solutions of similar past problems.

The general CBR process may be described by four tasks: RETRIEVE the most similar case or cases, REUSE the information and knowledge in that case to solve the problem, REINVENT (CREATE) the proposed solution, and RETAIN the parts of this experience likely to be useful for future problems.

**CBR Crucial Parts**

**FIRST PART**
- CASE representation
- SIMILARITY algorithm

**SECOND PART**
- ADAPTATION mechanism

**MIXING OF COMBINATORY PROBLEMS AND HEURISTIC SOLUTIONS**

- RAW MATERIALS CHEMISTRY
- RELATIONS BETWEEN CHANGES, CHEMICAL-PHYSICAL PROPERTIES AND PERFORMANCES
- ROLE, INFLUENCES AND RELATIONS BETWEEN INGREDIENTS
- COMPOUND/PERFORMANCES ASSOCIATIONS

**SHARING EXPERIENTIAL AND EPISODIC KNOWLEDGE**

- Race Engineer
- Compound Designer
- EPISODIC (NARRATIVE) KNOWLEDGE
- OLD CASE
  - Reuse
  - INNOVATION
- NEW CASE
  - New creation

**MIXING OF DATA AND UNCERTAINTY**

- ROAD GROUND
- TYRES DESIGN
- RADIO-TELEMETRY DATA
- CAR SET UP
- WEATHER CONDITIONS
- COMPETITORS benchmarking and weak points

**DECISION MAKING CYCLE**

- Grip
- Thermal Stability
- Mechanical Stability
- Warm Up

**Requirements of Performances**

- Chemical Formulation

**Daytona solution**

- Improvement to Thermal Stability without affecting Grip

**HSE20**

- New chemical formulation derived from HSE07

**ROAD GROUND AND CIRCUITS GEOMETRICAL PROFILE AND SEVERITY**

**WEATHER CONDITIONS**

**COMPETITORS**

**TYRES DESIGN**

**CAR SET UP**

**HISTORICAL DATA**

**CASE BASED REASONING**

**COGNITIVE PERSPECTIVE**

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**CBR Crucial Parts**

**FIRST PART**
- CASE representation
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**SECOND PART**
- ADAPTATION mechanism
Each CASE is a vector of attribute-value pairs.

Case solution: chemical formulation + race results

REVISE/ADAPTATION mechanism

How to MODIFY in the right way a rubber compound in order to get desired properties, without altering already good properties

What is the new chemical formulation satisfying the required performance

Abstract Compound Model (ACM)

Created for the representation and the computation of the chemical formulation of a compound as adaptation of previously developed products to new scenarios

Suitable for chemical formulations where basic ingredients in the formulation can be expressed with discrete quantities
ACM Rules: Activation Order

- Within each set, the choice of the rules determines how the recipe is revised in order to reach the desired performance.

CLASSIFICATION OF RULES

- **Description Rules**: describe a recipe of the company DB according to the ACM mode
- **Performances-Properties Rules**: define changes needed in the batch to obtain a required performance
- **Ingredients-Properties Rules**: define attributes of ingredients are involved in the adaptation
- **Formulation Rules**: rewriting rules that generate a the modified recipe ($R ightarrow R'$)

FORMULATION RULES

- **Substitution**: if $q_i \neq 0$; $i \in F_k$; $j \in F_k$; $|V_{ijk} - V_{ljk}| > T_{jk}$
  then
  $\{q_1, q_2, \ldots, q_{i-1}, q_i, q_{i+1}, \ldots, q_n\} \rightarrow \{q_1, q_2, \ldots, q_{i-1}, 0, q_{i+1}, \ldots, q_n\}$

- **Increase in quantity**: if $i \in F_k$ then
  $\{q_1, q_2, \ldots, q_{i-1}, q_i, q_{i+1}, \ldots, q_n\} \rightarrow \{q_1, q_2, \ldots, q_{i-1}, q_i + U_{ik}, q_{i+1}, \ldots, q_n\}$

- **Reduction in quantity**: if $i \in F_k$; $q_i > U_{ik}$ then
  $\{q_1, q_2, \ldots, q_{i-1}, q_i, q_{i+1}, \ldots, q_n\} \rightarrow \{q_1, q_2, \ldots, q_{i-1}, q_i - U_{ik}, q_{i+1}, \ldots, q_n\}$

Abstract Compound Machine (ACM) Model

Starting from a recipe $R$, a modified recipe is a recipe $R'$ where some quantities or ingredient type have been changed.

- Recipe of ingredients: $R = \{q_1, \ldots, q_n\}$ $q_i$ is the quantity of the ingredient $i$
- Each ingredient belongs to one or more families of ingredients
- Each family $F_k$ is described by a set $(a_{1k}, \ldots, a_{mk})$ of attributes
- Each ingredient is described by a value $V_{ijk}$ for each of its attributes $a_{jk}$
- $V_p = [V_{ijk} - T_{jk}, V_{ijk} + T_{jk}]$
  $T_{jk}$ is a constant of tolerance

CBR REVISE (ADAPTATION)

RETAIN (incremental learning)
Abstract Compound Machine - ACM

P-Race

P-Truck

COMPOUNDING PROBLEM

Searching based on IDA*

Genetic Algorithms

From PRace to PTruck: a more complex domain

P-Race

Tread for slick tires for race competitions

Different kind of BLEND USAGES:
- Segment (highway, road, quarries, multipurpose, ...)
- Truck axis (tractive, directional, trailer)
- Market (Italy, Turkey, Brazil, ...)
- a lot of Components (tread, liner, sidewall, ...)

The Compounding Problem: knowledge artifact approach

A set of requirements of modification of product characteristics

Proposal of the modification that fit better the set of requirements

P-Truck Compounding

Part of the P-Truck Project dedicated to the support of the compounding activity in the Business Unit Truck of Pirelli Tyres.

Rubber Blend Compounding: define the chemical formulation of rubber compound to be used in a truck tyre

Pirelli Experts in Compounding are Pirelli employees belonging to the Raw Material Division (chemistry experts) whose members study raw materials and how to combine and use them in truck tyres

The Knowledge Acquisition Campaign has been dedicated to the analysis of both the domain and the community of compounders

The group of compounders is a Community of Practice:
- Common objective and practices
- Shared language
- training of a new member
- transferring of experiences

The Acquired Knowledge:
- Domain Knowledge: which are the elements? And whose attributes? And relations among them?
- Adaptation Knowledge: which are the possible modifications? Do some constraints exists in modifying a blend?
- Problem Solving Method: how to use domain and adaptation knowledge in order to give an effective support to the user

Design by Adaptation: how to modify a previously solution in order to obtain the most suitable blend for the current problem

The actual support: proposal of the modification that fit better a set of requirements of modification of product characteristics

Pirelli Tyres
Recipe Modifications vs. ACM Formulation Rules

**Recipe Modifications**
- Substitution for Discrete Attribute
- Substitution for Continuous Attribute
- Substitution for Family Type Variation

**ACM Formulation Rules**
- Increase in quantity
- Reduction in quantity

**Ingredients' Ontology**
- Types and Families of Ingredients

**Lab Test Results**
- Static Conditions
- Dynamic Conditions
- Durability Tests
- Seniority

**Low-level, and High-level properties of a rubber compound**
- Lab Tests
- Outdoor Tests
T-Matrix Knowledge Artifact

T-Matrix is an explicit representation of known but implicit relationships between domain entities held by expert compounders involved in the compounding problem.

Describing the T-Matrix: Recipe Modifications

- Substitution with Family Type Variation
  - Substitution of Carbon Black (Structure increase)
- Substitution with Continuous Attribute Variation
  - Addition of Natural Rubber (in increase)
- Substitution with Discrete Attribute Variation
  - Addition of Sulphur Rubber (a decrease)

Describing the T-Matrix: Tyre Performances

- Dry Rolling
- Wet Handling
- Fading
- Tread Resistance (sidewall breakdown)
- Tear Regularity

The Compound Modification Theory

In correspondence with all the possible entries, we find relations qualified with regard to:

- Correlation (X, Y, Z) could be Strong, Good, Weak or Null
- Proportionality (X, Y) could be Direct or Inverse

How T-Matrix can be read

[First Step] The specification of the desired compound performance
- Strong increase of Tread Tear Resistance

[Second Step] The translation in characteristics values (coming from lab tests)
- Strong increase of Elastic Dynamic Modulus; show increase of Low Sevity Abrasion; Wear decrease of hysteresis

[Third Step] Searching for the correspondent structural modification actions
- Augmentation of Sulphure Rubber amount
- Removal of Carbon Black amount
- Addition of Natural Rubber amount
- Removal of Zinc amount
**Abstract Compound Machine - ACM**

Ida* searching based on the T-Matrix.

**Knowledge Artifact (T-Matrix)**

The designed computational model is an instantiation of the Iterative Deepening A* (IDA*) algorithm, with respect to the ontological knowledge on the problem.

**Effects**

Abstract Compound Machine - ACM

**Constraints**

Due to the basic compositional features of the Chemistry Formulation Problem, the actual implementation has been made within the State Space Search computational paradigm.

**The Compounding Problem:**

Searching in the space of requirements of modification of product characteristics.

**Automatic generation of a new recipe**

**Constraints**

The ontological analysis furnished a deep and formalized understanding of the rubber compound structure.

**The constraints**

imposed a set of domain-dependent constraints on the pre-conditions of the transitions between states.

The constraints reduce considerably the state space dimension and, consequently, improve the computational efficiency of the evaluation phase of the new states (at each expansion step).
Blend Features Modifications

**STRONG Augmentation**
- e.g. Tensile Strength (TS)

**WEAK Augmentation**
- e.g. High Severity Abrasion (HSA)

An appropriate metric has been developed with respect to each low-level and high-level property in order to manage lab test results:
- e.g. "Tensile Strength":
  - WEAK = 2.50%
  - GOOD = 7.50%
  - STRONG = 10.00%

**Exploring the Solution Space: IDA***

- **A* Search**
  - Takes both the path to a node and the heuristic into account.
  - Let $g(n)$ be the cost of the path found to node $n$.
  - Let $h(n)$ be the estimate of the cost from $n$ to a goal.
  - Let $f(n) = g(n) + h(n)$, which is an estimate of the cost from the start to a goal via $n$.

- **Iterative Deepening A* Search**
  - Memory bounded $A^*$ algorithm.
  - Each iteration is a depth search with limit cost function $f(n)$.

**Linking the search spaces: T-matrix**

In correspondence with all the possible entries, we find relations qualified with regard to:
- Correlation (\$\{, \$\} could be Strong, Good, Weak or Null)
- Proportionality (\$\$) could be Direct or Inverse

An appropriate metric has been developed with respect to each low-level and high-level property in order to manage lab test results:
- e.g. "Tensile Strength":
  - WEAK = 2.50%
  - GOOD = 7.50%
  - STRONG = 10.00%

- e.g. "Hardness":
  - WEAK = 0.75%
  - GOOD = 2.25%
  - STRONG = 3.00%
Test [II]: Aumento manovrabilità asciutto e bagnato

Test [III]: Aumento resistenza al rotolamento

Abstract Compound Machine - ACM

L. Int. Ar. approach to Compounding

Knowledge Artifact (T-Matrix)

Search based on IDA*

Genetic Algorithms

The Compounding Problem: Following the evolutionary metaphor

(EVOLUTIVE) GA APPROACH

Final Population of recipes

Fitness function: multi-criteria comparison of compound properties

- Population of recipes?
- Population of modification actions?