**European Innovation Partnership on Raw Materials**

**Application for a Raw Materials Commitment**

**Simulation and development of innovative hydrometallurgical processes for the valorization of low grade and polymetallic resources**

**Acronym:** SX-dev

**Links to the Strategic Implementation Plan:**

- I. Technology Pillar
  - I.B Priority Area: Technologies for primary and secondary raw materials’ production
    - Action area n° I.4: Processing and refining of raw materials
      - 2) Metallurgical systems

**Objectives of the commitment:**

The development of green technologies based on novel materials which are essential to meet the needs of expanding populations is placing great demands on mineral resources. Easy to access resources are depleting and hydrometallurgy has the technical and economic potential to recover valuable metals from complex and low-grade resources (primary and secondary). Amongst other benefits, hydrometallurgy contributes to resources efficiency policies thanks to the valorization of the maximum of metals contained in a resource. In this framework, the present project is focused on the improvement of the performances of one of the most frequently used technologies in modern hydrometallurgy: solvent extraction. The development of databases, simulation and new extractant molecules adapted to more complex ore or waste matrices will induce the enhancement of the performance of the overall metallurgical process

**Description of the activities:**

Solvent extraction is a mature separative technology based on a phase transfer process between an aqueous phase and a non-miscible organic phase to selectively and reversibly recover valuable metals. During the operation of Solvent eXtraction (SX) plants, changes in ore composition or solvent ageing can lead to a dramatic drop of the process efficiency and the quality of the product. Greater control of the process chemistry and optimization of the operating conditions are essential to ensure a high level of performance.

The chemistry of the process can be improved by optimizing the solvent formulation. In particular, most commercially available extractants were developed more than 20 years ago and are not
suitable to treat “pregnant leach solutions” (PLSs) obtained from polymetallic and low-grade ores. The challenge in this project is to design new molecules that can extract strategic metals from PLSs that contain low concentration of valuable metals and many impurities at high concentration. The program employs a rational approach based on the use of transverse skills offered by the consortium: (i) physicochemistry to understand the chemical phenomena involved in SX, (ii) molecular modeling to define the effects of the structures of extractants and the diluents on the strength and selectivity of metal extraction, (iii) synthetic organic chemistry at laboratory and plant scales to obtain technocommercially viable extractants and (iv) chemical engineering to develop flow sheets and to optimize metal separation and recovery.

The optimization of the SX parameters and the prediction of the process behavior in case of variation of operating conditions (redox potential, resource composition, pH, etc.) are important to obtain good material and energy balances in the system. Consequently, the development of a simulation tool able to predict the performance of the SX component of the flow sheet is essential. To our knowledge, such tools are not available for hydrometallurgy and their usefulness relies on a precise description of the physicochemistry involved in SX from the molecular to the thermodynamic levels. Several modules are contemplated.

The first module contains databases which feed the second: thermodynamic calculations (speciation and mass transfer at the liquid-liquid interface). The program MT-Data will be used to predict the speciation in solution by using a reliable database containing Pitzer parameters for activity coefficients calculations, thermodynamic stability constants and extraction constants. Mass transfer calculations at the liquid-liquid interface will be possible by developing a model describing the physicochemistry involved during SX. All of the data from the second module will feed the third, based on the Usim Pac software (Caspeo), which will be modified to include chemical engineering algorithms to predict the behavior of SX processes and to optimize the operating conditions and the flow sheets. The simulation tool and the flow sheets will then be validated in pilot trials.

The project has been organized in different tasks and its successful achievement relies on strong interaction between all partners as described in the partnership.

This strategy will be applied to the recovery of nickel and cobalt from lateritic ores which, despite representing more than 60% of nickel reserves, have so far been largely untreated. The methodologies generated in the programme will underpin the development of processes to recover other strategically important metals, including those which can be sourced by “urban mining”.

**Description of the expected impacts:**

The overarching aim of the project is to secure raw materials supply to Europe by maximizing significantly the efficiency of hydrometallurgical processes for metal-recovery from low grade mixed metal ores and waste materials. Within this framework, this project relies on the implementation of simplified and optimized flowsheets thanks to the development of a simulation tool and the use of new extractant molecules specifically designed for these flow sheets. The rational approach and the tools developed in this project will firstly be applied to the recovery of nickel and cobalt contained in laterite ores, which have so far been largely untreated. However, this research program could be extended to the development of new processes for the recovery of strategic metal from other primary and secondary resources such as the extraction of lithium from brines by exploiting the very high selectivity which is possible in solvent extraction processes using appropriately designed reagents or the recovery of strategic metals from spent batteries (nickel, cobalt, lithium), spent LEDs and WEEE.

The science and technology arising from the project will benefit European researchers in industry and academe well beyond those working with metals. The computational methodologies will have impact on separation sciences in general, a research area which has been poorly funded in many European states in the last two decades. The understanding of the chemistry which results in very high selectivity of metal solvent extraction impacts on a number of areas of great topical interest.
such as effluent processing, environment and health, extractive metallurgy, etc.

**Expected innovation outcomes:**
New products to the market
New processes

**Comments:**

As described above, the innovation of the project provides:
- A rational approach to develop environmental friendly innovative processes for the recovery of strategic metals from mining and urban mining resources which will underpin the secure supply of key metals. The collaboration involved in the project also provides for the commercial development of extractants for hydrometallurgical processes to treat new polymetallic and low grade ores (the last commercial reagents for cobalt and nickel were developed more than 20 years ago).
- New simulation tools for use in hydrometallurgy. There are currently none to simulate solvent extraction processes. Among other, Aspen-Hysis is a powerful software but the thermodynamics and the database are not adapted to hydrometallurgical processes. Likewise, CEA is developing a simulation tool to simulate solvent extraction processes but it is dedicated to fuel reprocessing.

**Name of the coordinating organisation:**
ERAMET Research

**Country:**
France

**Entity profile:**
Private sector - large company

**Role within the commitment:**
ERAMET Research is a subsidiary of ERAMET group, a French mining and metallurgical company. ERAMET Research works on improving existing metallurgical processes and developing new ones. Eramet will bring its expertise in the development of hydrometallurgical processes to develop the simulation tool in collaboration with Partners 3 and 6. ERAMET will also give their expertise for designing economic and performant flow sheets in collaboration with Partners 2, 7 and 8.

**Other partners:**

**Name of partner:**
ENSCP-IRCP

**Country:**
France

**Entity profile:**
Academia

**Role within the commitment:**
This team works on solvent extraction to improve or develop efficient processes. They will develop physicochemical models with Partner 5 to describe metals transfer at the liquid-liquid interface. Such models will be included in the simulation tool in collaboration with Partner 3. They will also work on the design of extractant molecules with Partners 2, 4 and 8 and their implementation in flow sheets with Partners 1 and 7.

**Name of partner:**
ICMUB

**Country:**
ICMUB is specialized in organophosphorus chemistry and they work on the synthesis of new extractants for uranium recovery in collaboration with Partner 2 for 5 years. They will use their expertise to develop new synthesis pathways of extractants so that the synthesis will be easily scaled-up. The choice of the molecules structures will be the results of the investigations carried out by partners 4, 5, and 8 especially for the scale-up.

Name of partner: CASPEO
Country: France
Entity profile: Private sector - SME
Role within the commitment:
Caspeo develops the USIM PAC software tool, a steady-state simulator that allows modelling and simulation of mineral processing for design and optimisation. The thermodynamic database, the physicochemical models and the speciation module developed in the present project will be introduced to the existing library of SX mathematical models. The platform will then be used to design and optimise the full hydrometallurgical flowsheet including upstream and downstream unit operations.

Name of partner: University of Edinburgh
Country: United Kingdom
Entity profile: Academia
Role within the commitment:
They will work with Partners 1, 2 and 8 to design new extractants. In particular, they will investigate the influence of the nature of the diluent and the structure of the extractant molecules on the extraction properties as well as the stability of metal-ligand species in aqueous and organic phase by means of molecular modeling. This part of the project will be useful to help the physicochemist to determine metal speciation.

Name of partner: Chalmers University
Country: Sweden
Entity profile: Academia
Role within the commitment:
Chalmers has been working for more than 50 years in solvent extraction processes. With
Partner 6 will focus on the development of thermodynamic data for speciation calculations in aqueous phase by using/determining activity coefficients, stoichiometry and thermodynamic constants of formation of metal-ligand complexes. With Partner 1 will focus on the extraction properties of extractants and the investigation of the influence of the diluent on extraction properties.

**Name of partner:**
MIRO

**Country:**
United Kingdom

**Entity profile:**
Private sector - SME

**Role within the commitment:**
A key aspect of this project will be the simulation of the system chemistry and MTDATA is the preferred model with which this will be achieved. The technical contribution will be split jointly between three activities: (1) Data collection and assessment; combining commissioning and interpretation of new experimental data from this project, its formal assessment and incorporation into pre-existing data sets. This will include a continuous task of model and database testing and will be in co-operation with partner 5. (2) Optimisation of developing industrial processes; new technologies will be explored during this project and thermodynamic simulation will be essential in their development and assessment, in order to maximize process yield and minimise both energy consumed and waste generated (3) Integration of MTDATA with other numerical tools for process control, development and testing. MTDATA will form the core chemical speciation and phase equilibrium code in a larger, coupled simulation package. The integration of two (or more codes) into a bespoke system model is a multi-partner task to which MIRO and NPL will contribute in co-operation with Partners 1 and 3

**Name of partner:**
IMN

**Country:**
Poland

**Entity profile:**
Governmental/public body

**Role within the commitment:**
They will validate the simulation tool developed in this project by means of pilots. This tool will then be used to design an optimized flow sheet for the recovery of cobalt and nickel from laterites ores or other valuable metals from other complex matrices (mining or urban mining). For these goals, they will work closely with Partners 1, 2 and 8.

**Name of partner:**
CYTEC

**Country:**
United States

**Entity profile:**
Private sector - large company

**Role within the commitment:**
Cytec develops and manufactures extractants and help hydrometallurgical companies to implement them in their processes. This team will bring its expertise to develop extractants and flow sheets with Partners 1, 2 and 4. They could also potentially assist with the piloting at semi-scale level (mini-rigs) of the most promising extractant molecules with synthetic or real feed metal solutions on site at one of their facilities in Canada or the US.

**Existing EU contribution:**
No

**Period to implement the commitment:**
Sunday, 1 March, 2015 to Friday, 1 March, 2019