



Modelling and simulation of molybdenum extraction by HDEHP ion-exchanger and DMDOHEMA solvating extractant

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Modelling and simulation of molybdenum extraction by HDEHP ion-exchanger and DMDOHEMA solvating extractant

ISEC 2014 – Nuclear Chemistry For Sustainable Fuel Cycles | V. Vanel, C. Marie, M. T. Duchesne, X. Hérès, V. Pacary, L. Berthon, D. Rudloff, M. Bertrand, S. Watanabe

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Introduction

The EXAm process and the Mo stripping step
How does the Mo stripping step work?
Approach adopted to build the model

Modelling of Mo behavior

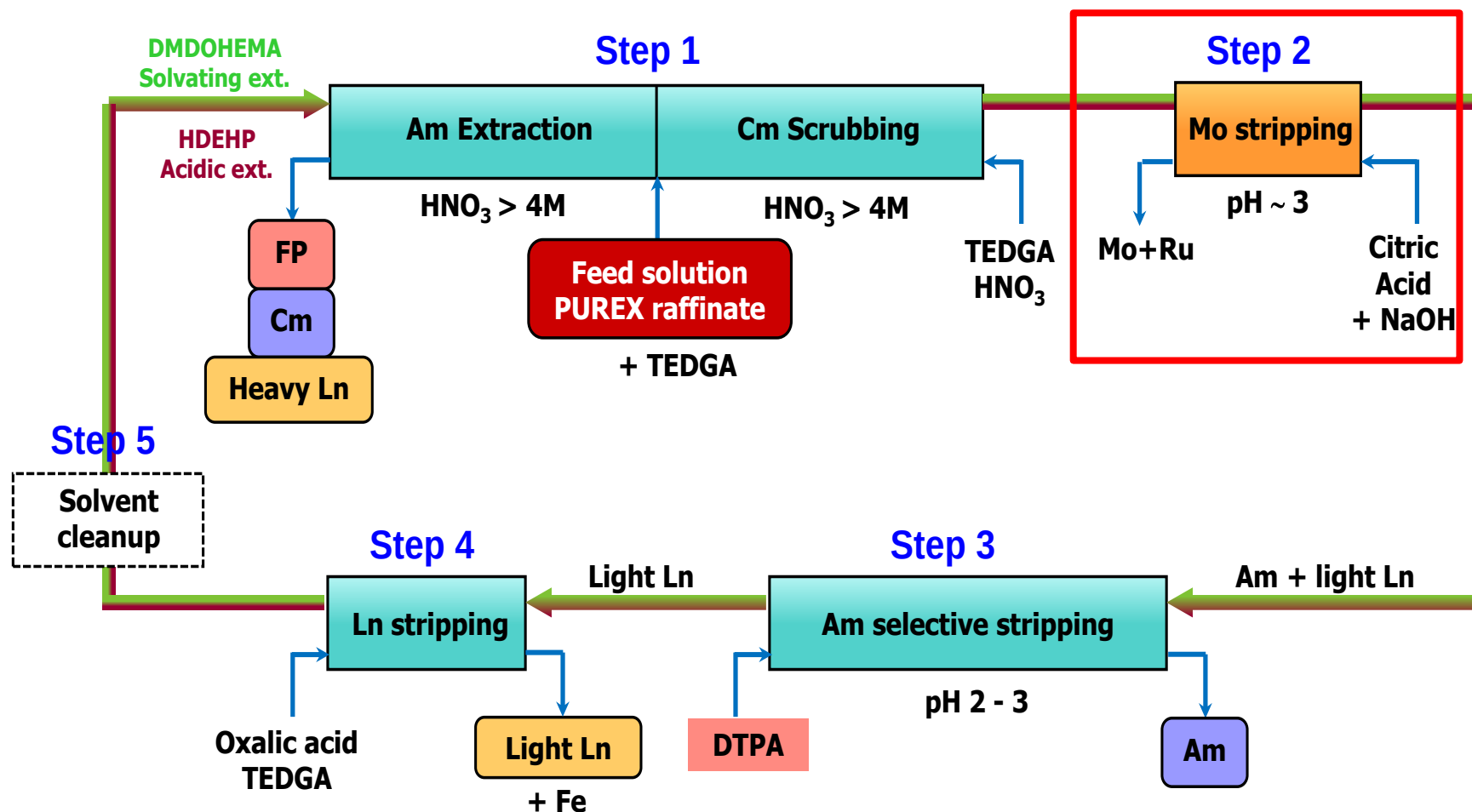
Comparison with experimental results

Batch experiments
Implementation in the PAREX code
Cold tests (G1 facility, Marcoule)

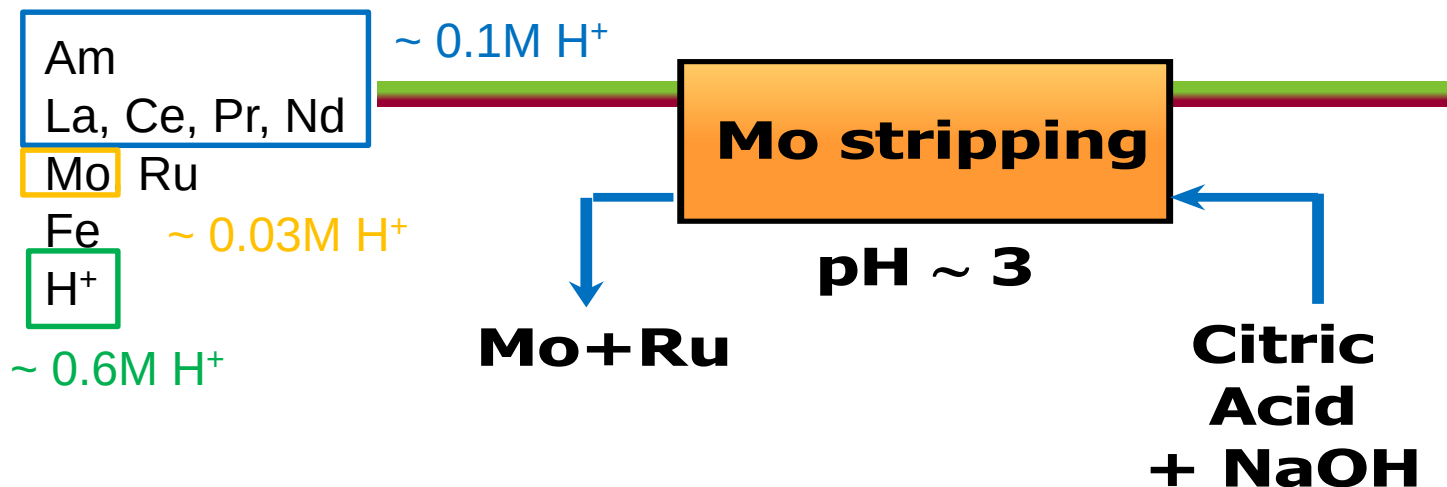
Conclusion - prospects

The EXAm process and the Mo stripping step

- The EXAm process aims at recovering americium alone from the PUREX raffinate



How does the Mo stripping step work?



Change from an acidic medium (4 – 5 M) to weak acidic conditions (pH 2 – 3)
Neutralization of extracted acid by NaOH

Recombination of extracted complexes in the organic phase
4 – 5 M: predominant effect of DMDOHEMA (solvating extractant)
pH 2 – 3: predominant effect of HDEHP (cationic exchanger) $\Rightarrow$ release of H⁺

Citric acid: complexing power vs. acid buffer

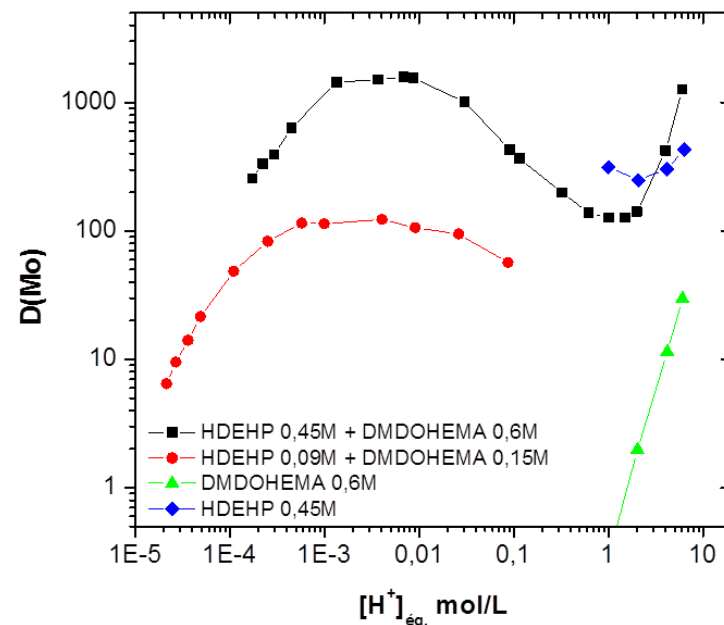


Stripping of Mo

Approach adopted to build the model

■ Determination of constants on batch experiments

Reference : Marie C., Watanabe S., Vanel V., Duchesne M.-T., Zorz N., Berthon L. Behaviour of Molybdenum (VI) and Iron(III) in {HDEHP-DMDOHEMA-nitric acid} liquid-liquid extraction systems. Paper in preparation

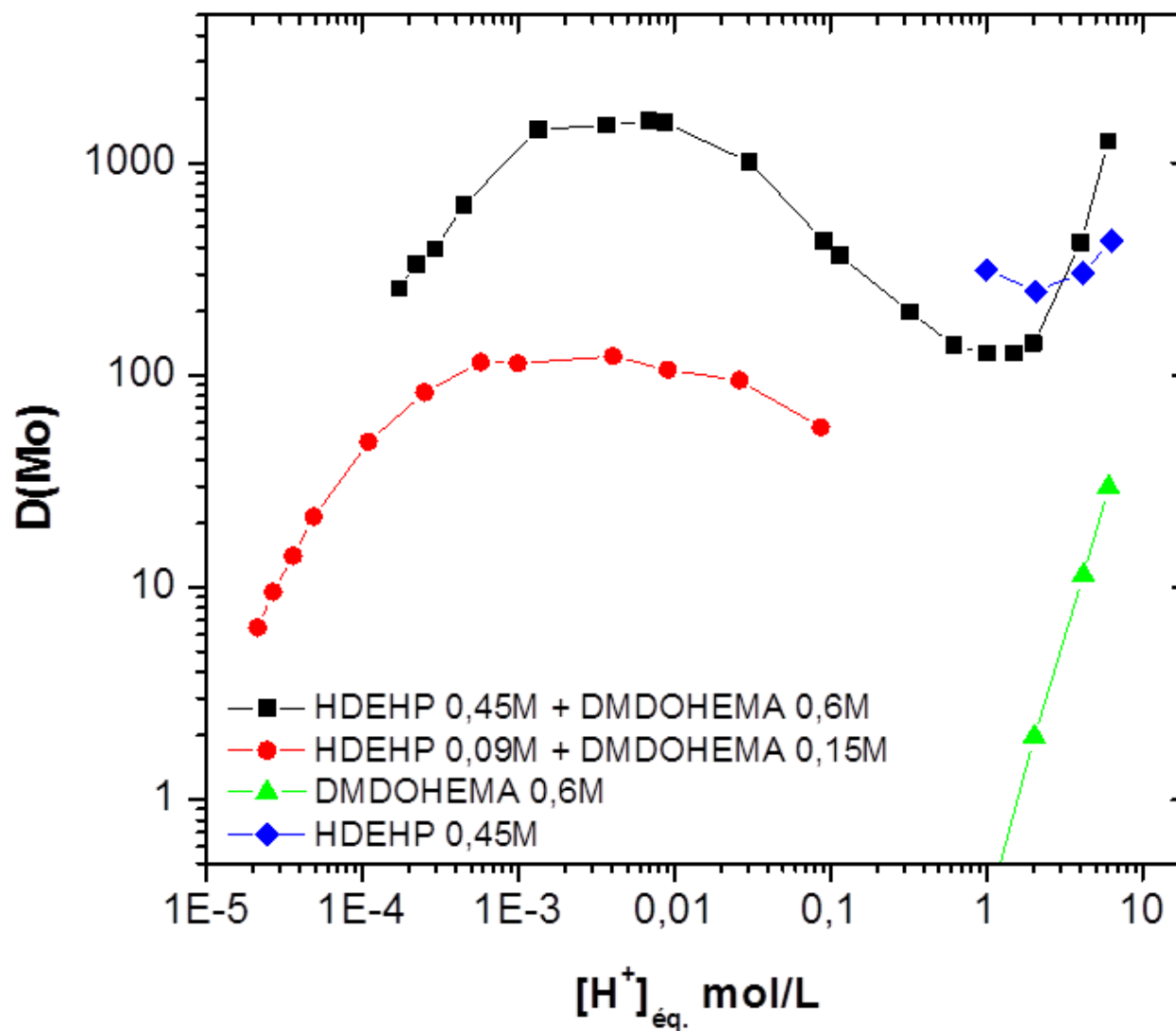


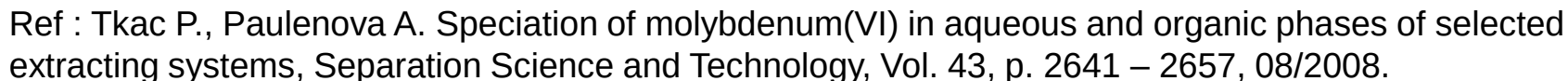
■ First validation of the model on a cold test (G1 facility at Marcoule)

Reference : ???

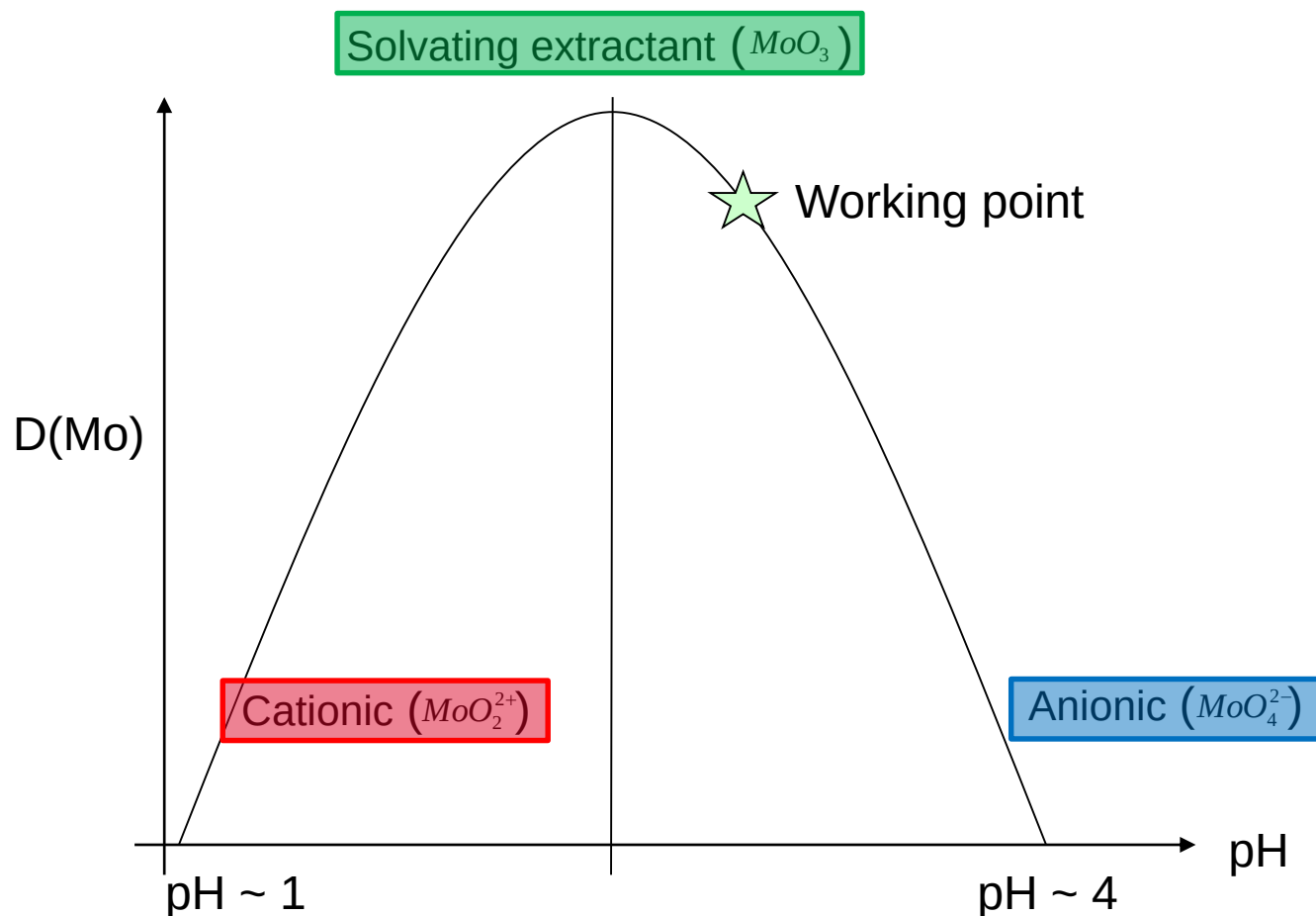


Modelling of Mo(VI) behavior





Modelling of Mo(VI) behavior

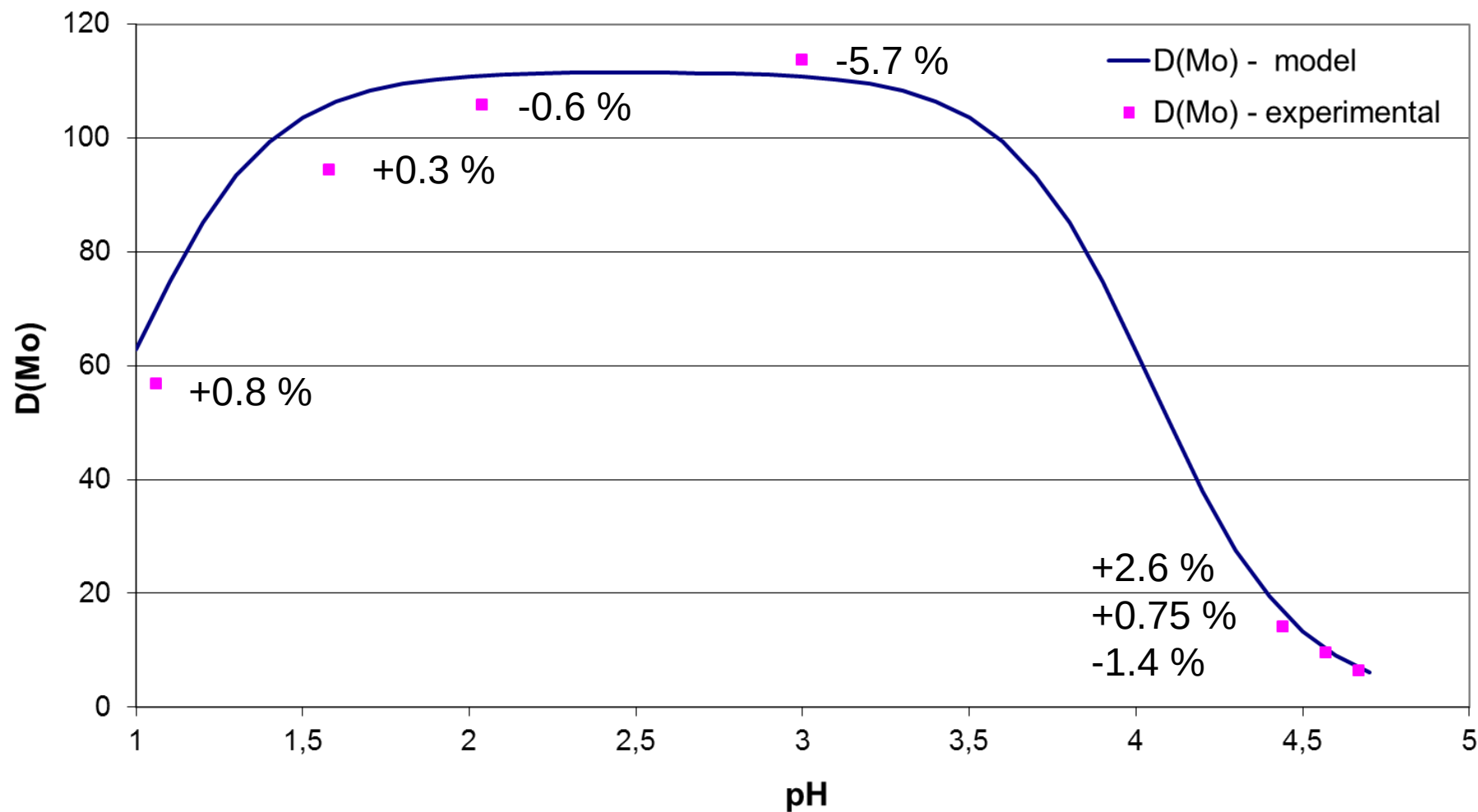


Ref : étude d'un procédé de valorisation du molybdène par extraction par solvant organophosphore, C. Brassier, thèse CEA-R-5689, 1995

Modelling of Mo(VI) behavior

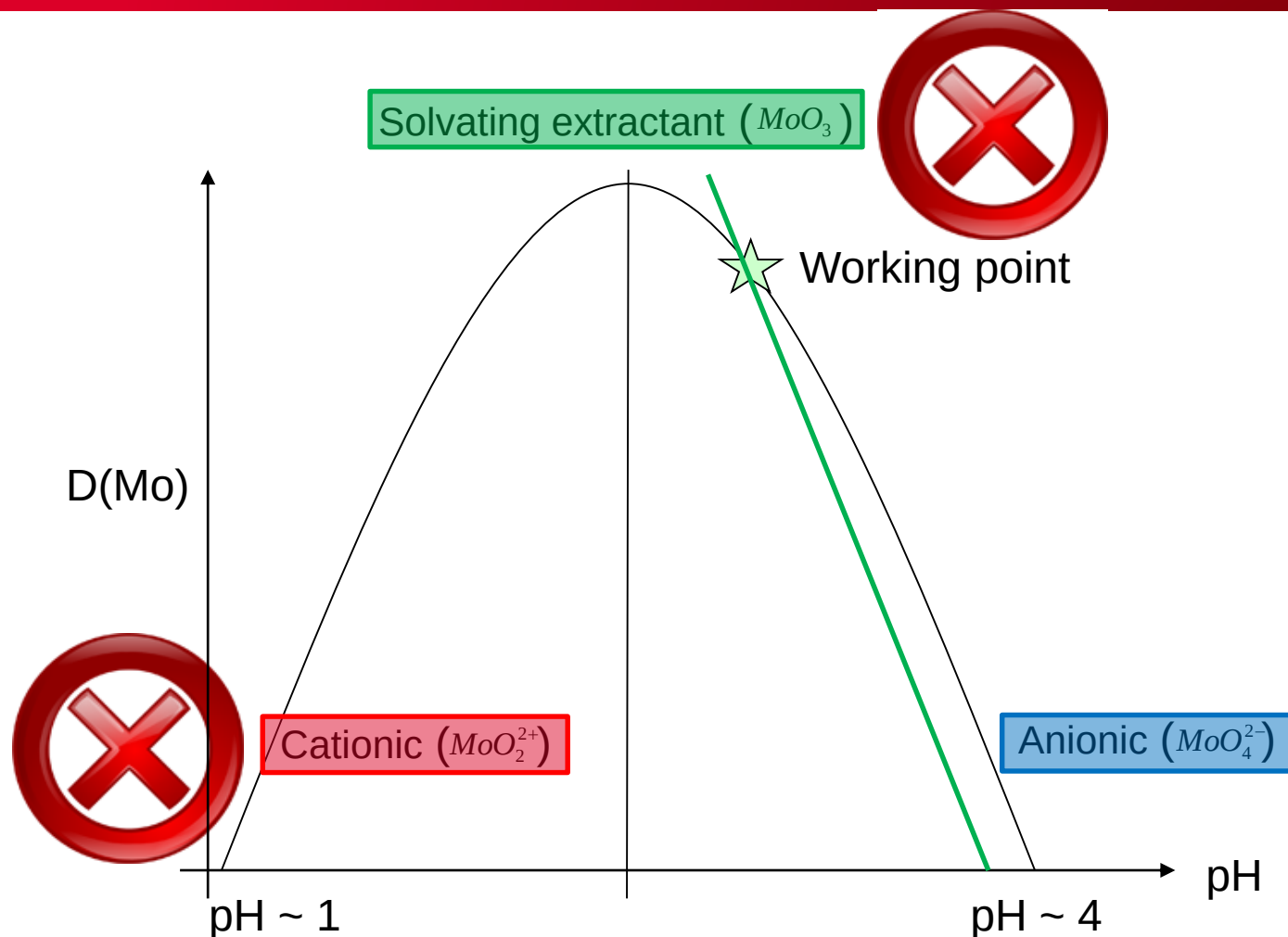
Chemical reaction	Formula	Log(K)
MoO_2^{2+} / MoO_3	$[MoO_2^{2+}] = K(MoO_2^{2+} / MoO_3) \times [MoO_3] \times [H^+]^2$	1.9
MoO_3 / MoO_4^{2-}	$[MoO_3] = K(MoO_3 / MoO_4^{2-}) \times [MoO_4^{2-}] \times [H^+]^2$	8.1
Cation exchanger	$[MoO_2 DEHP_2 HDEHP_2] = K_{ec} \frac{[MoO_2^{2+}] \times [HDEHP]^4}{[H^+]^2}$ 	4.7
Solvating extractant	$[MoO_3 HDEHP_4] = K_{es} \times [MoO_3] \times [HDEHP]^4$ 	5.5
Anion exchanger	$[MoO_2 DEHP_2 HDEHP_2] = K_a \times [MoO_4^{2-}] \times [HDEHP]^4 \times [H^+]^2$ 	13.6

Modelling of Mo(VI) behavior

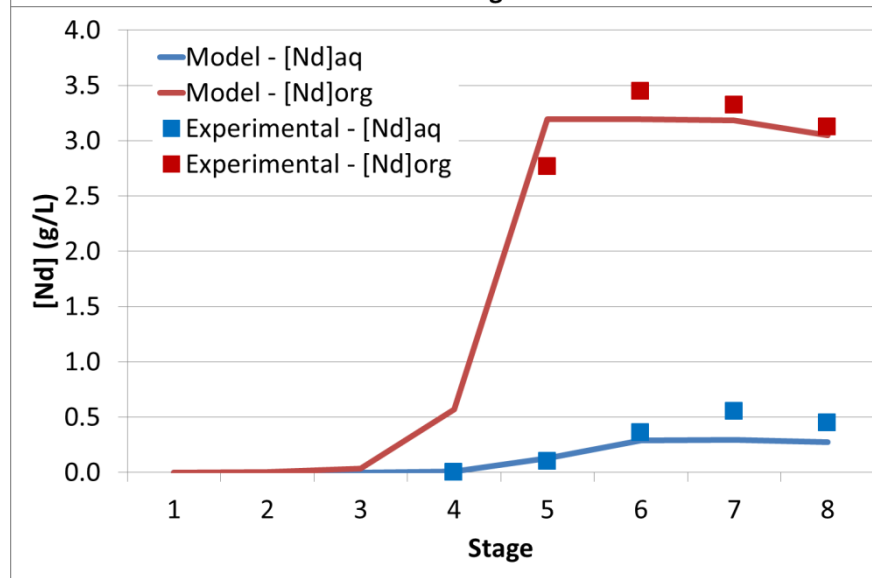
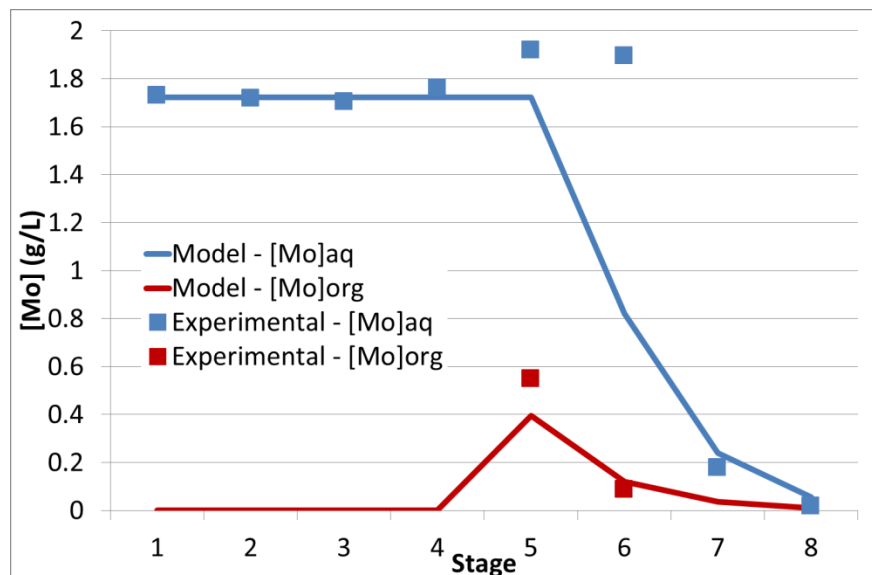
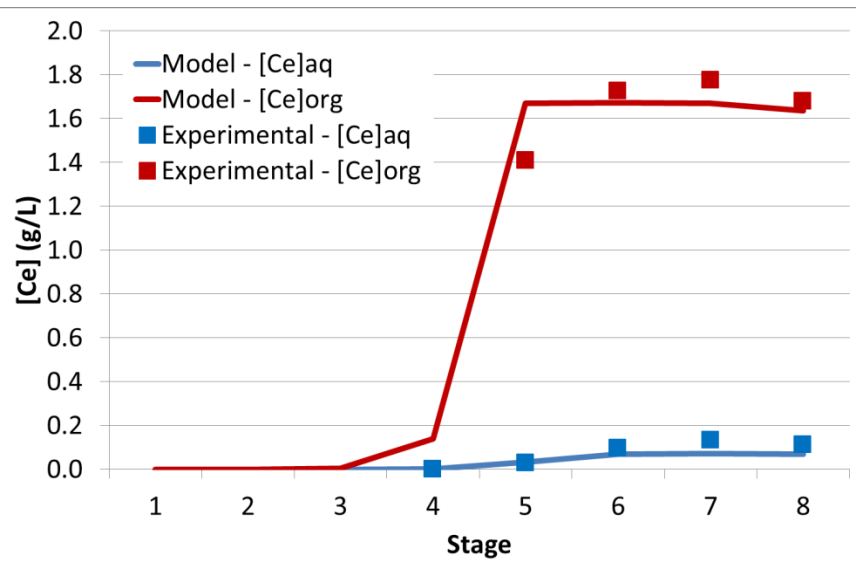


Model seems to be representative of Mo behavior

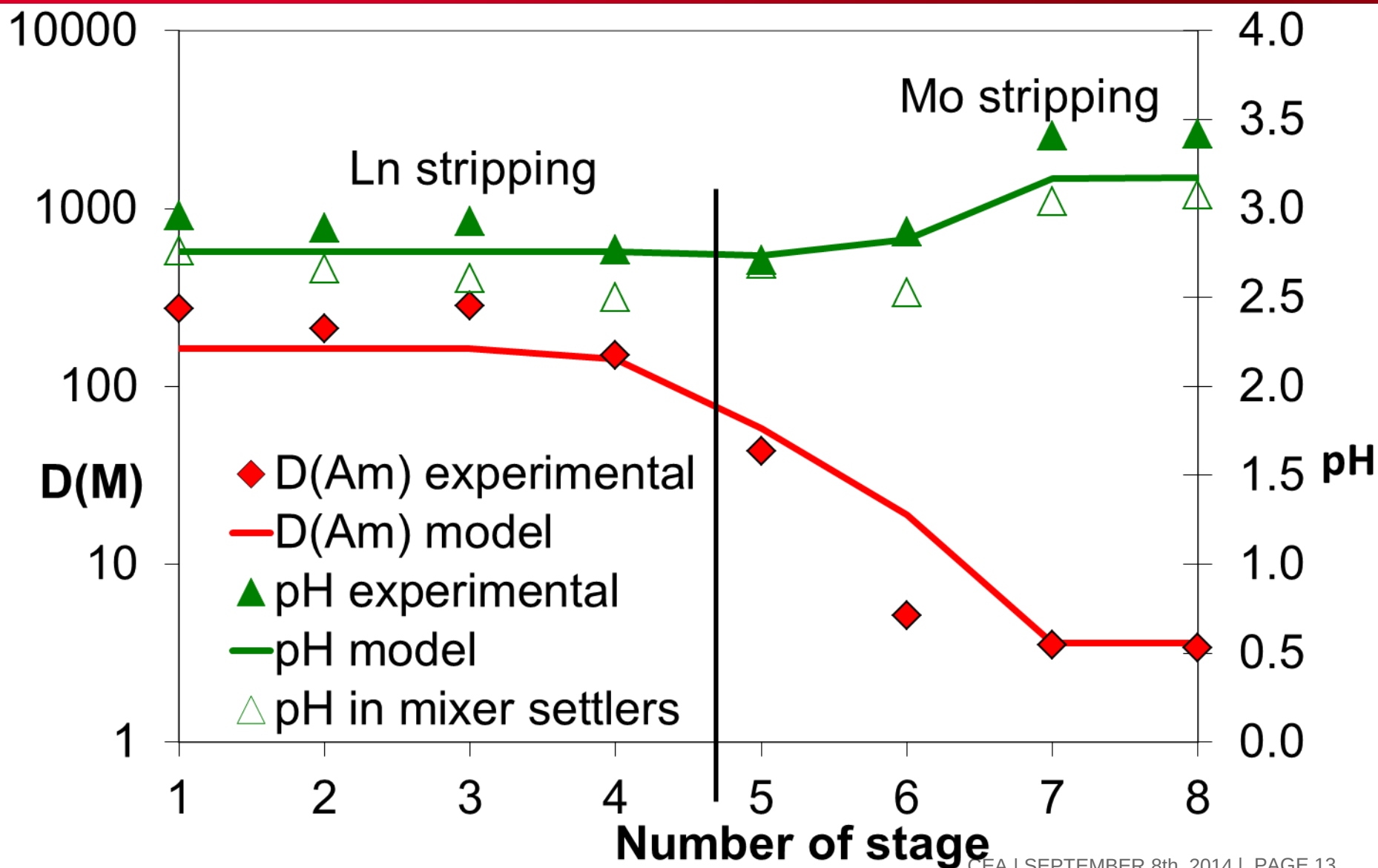
Implementation in the PAREX code



Cold test (G1 facility, Marcoule)



Cold test (G1 facility, Marcoule): trace amounts of Am



Conclusions - prospects

■ Conclusions :

- Modelling quite representative for Am, La, Ce, Pr, Nd and Mo in weak acidic conditions
- Use of models to propose flowsheets for hot tests, both in trace and macroscopic amounts of actinides.

■ Prospects :

- Implement the complete model in the PAREX code
- Compare the model to future hot tests (trace and macroscopic amounts of actinides)



Thank you for your attention!



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