



**HAL**  
open science

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

V Vanel, C Marie, M T Duchesne, X Hérès, V Pacary, L Berthon, D Rudloff, M Bertrand, S. Watanabe

### ► To cite this version:

V Vanel, C Marie, M T Duchesne, X Hérès, V Pacary, et al.. Modelling and simulation of molybdenum extraction by HDEHP ion-exchanger and DMDOHEMA solvating extractant. ISEC 2014 - 20th International Solvent Extraction Conference, Sep 2014, Würzburg, Germany. cea-02997814

**HAL Id: cea-02997814**

**<https://cea.hal.science/cea-02997814v1>**

Submitted on 10 Nov 2020

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

DE LA RECHERCHE À L'INDUSTRIE



# 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. Hérés, V. Pacary, L. Berthon, D. Rudloff, M. Bertrand, S. Watanabe

[www.cea.fr](http://www.cea.fr)

Monday, September 8th, 2014



## 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

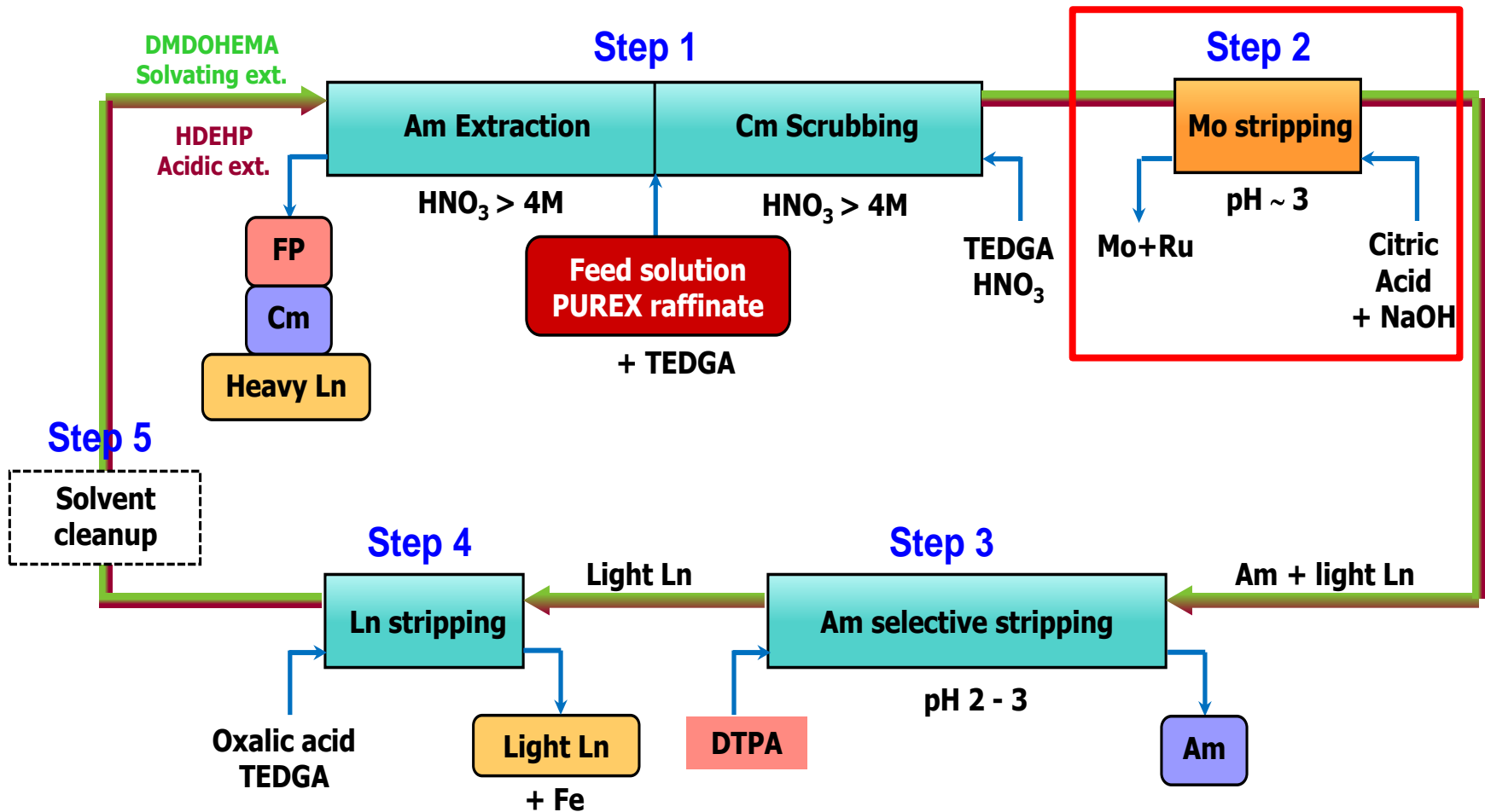
## Comparison with experimental results

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

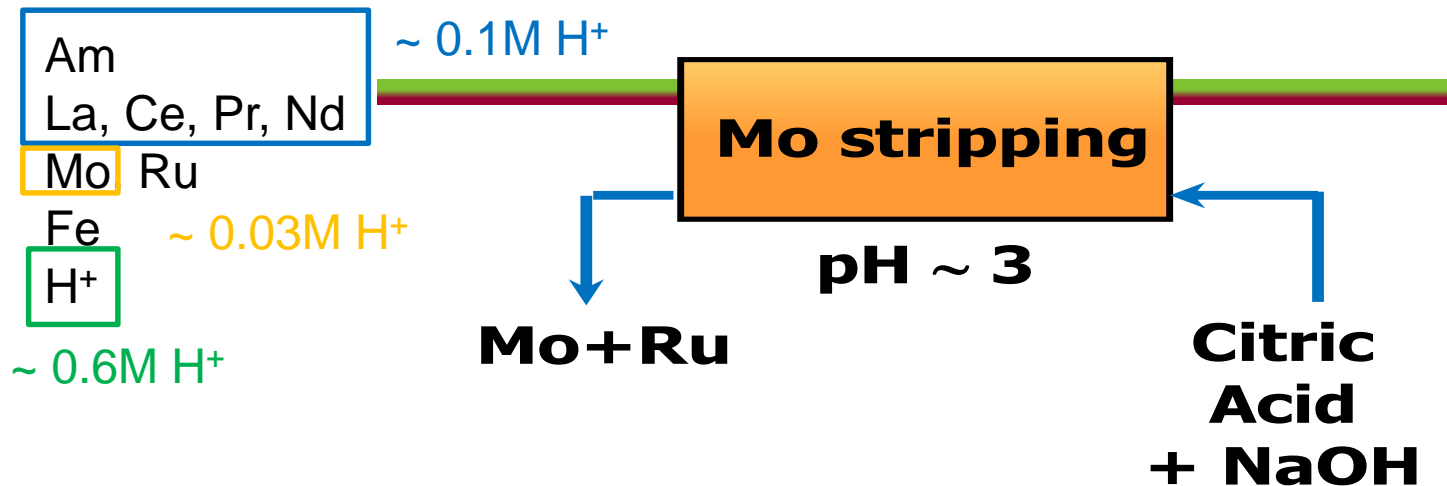
## Conclusion - prospects

# 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) => release of H<sup>+</sup>

Citric acid: complexing power vs. acid buffer

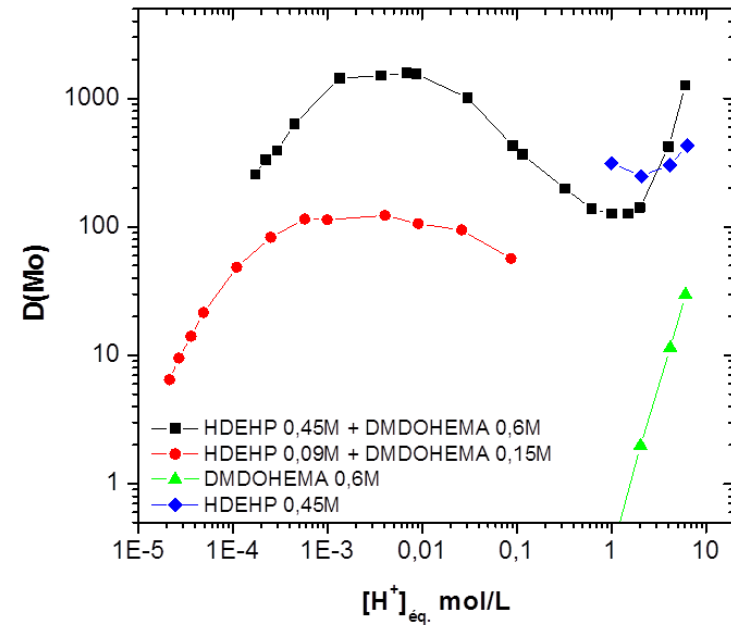


Stripping of Mo

# 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

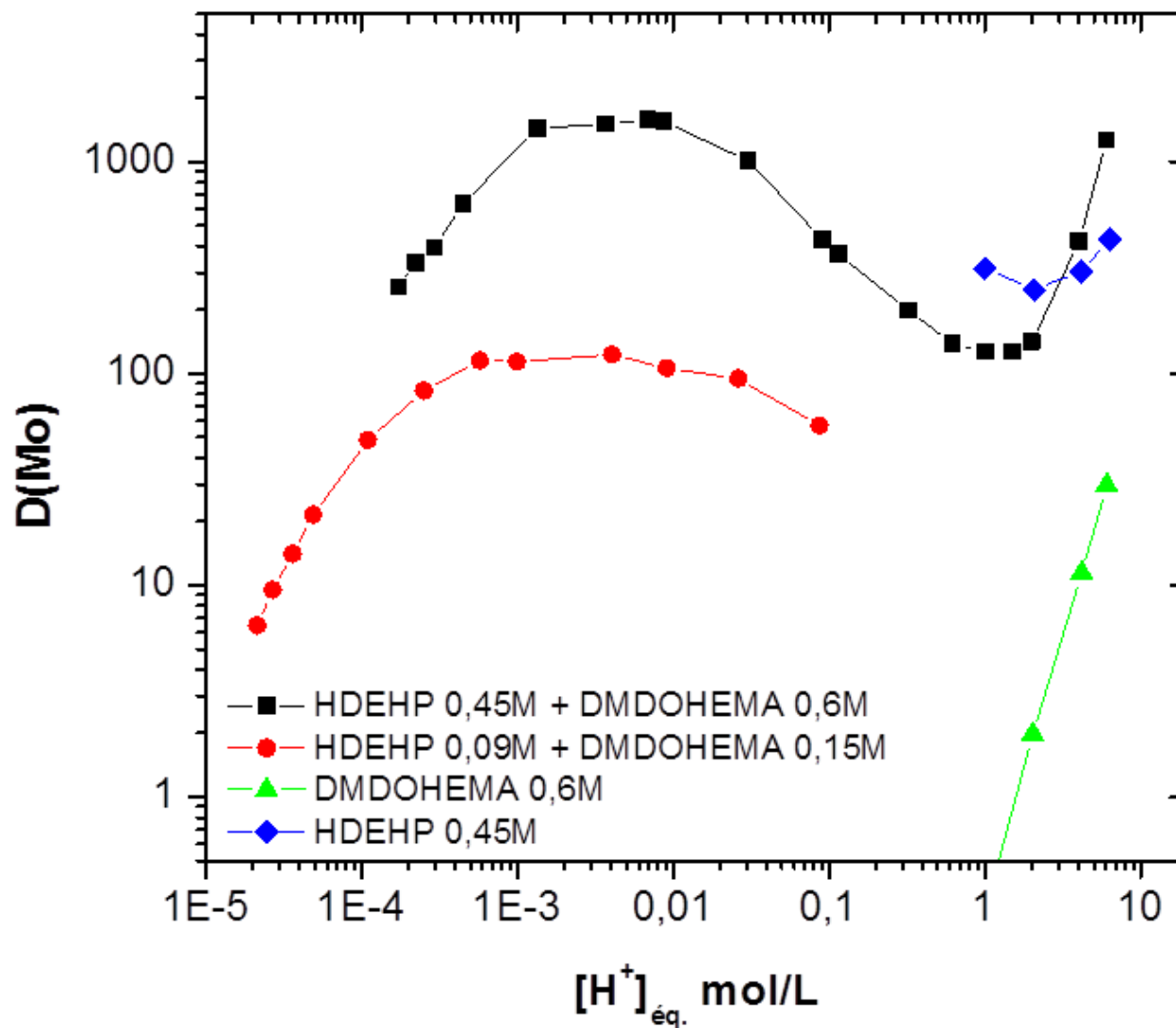


- First validation of the model on a cold test (G1 facility at Marcoule)

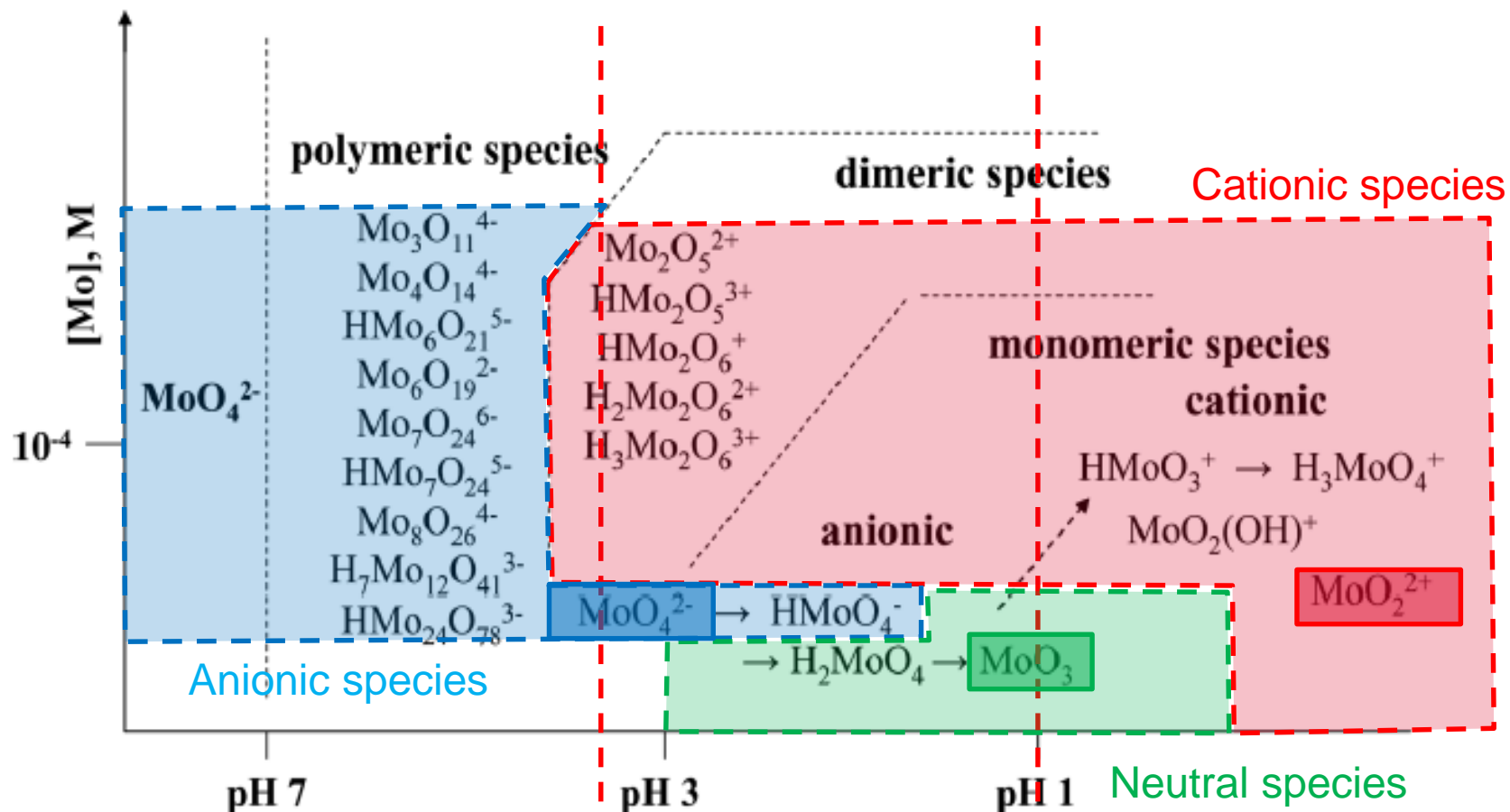
Reference : ???



# Modelling of Mo(VI) behavior



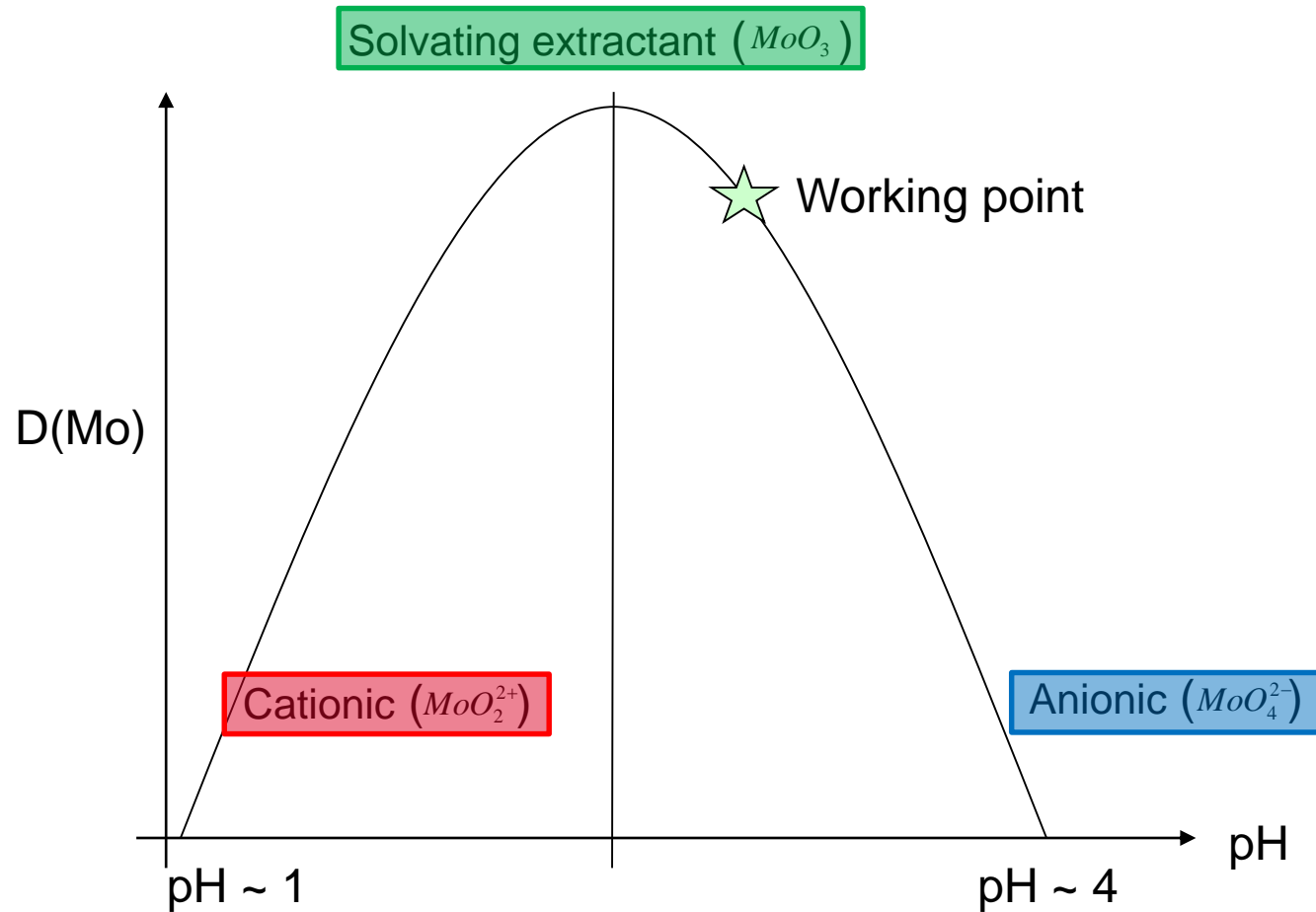
# Modelling of Mo(VI) behavior



Ref : Tkac P., Paulenova A. Speciation of molybdenum(VI) in aqueous and organic phases of selected extracting systems, Separation Science and Technology, Vol. 43, p. 2641 – 2657, 08/2008.






# Modelling of Mo(VI) behavior

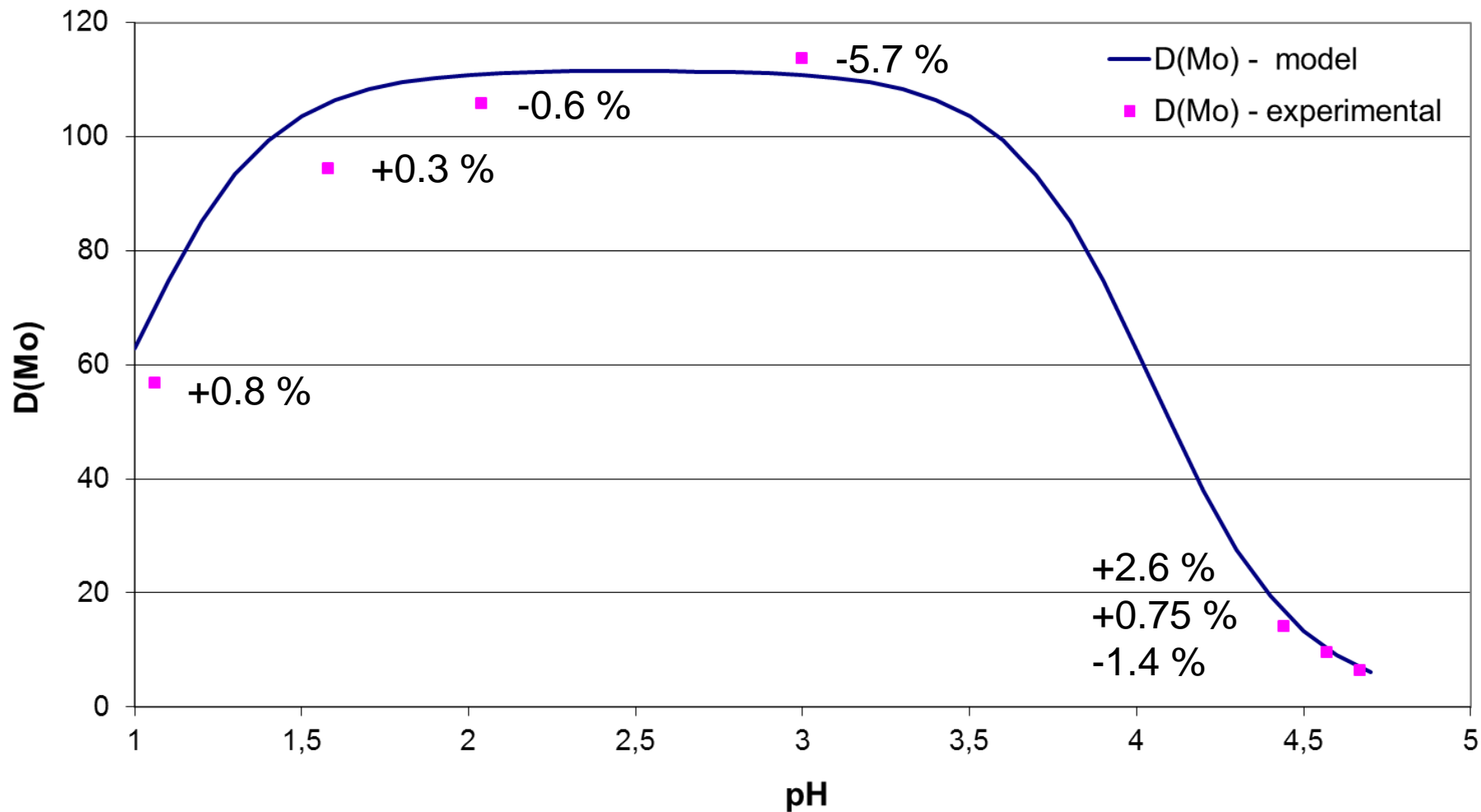


Ref : étude d'un procédé de valorisation du molybdène par extraction par solvant organosphosphore, C. Brassier, thèse CEA-R-5689, 1995

# Modelling of Mo(VI) behavior

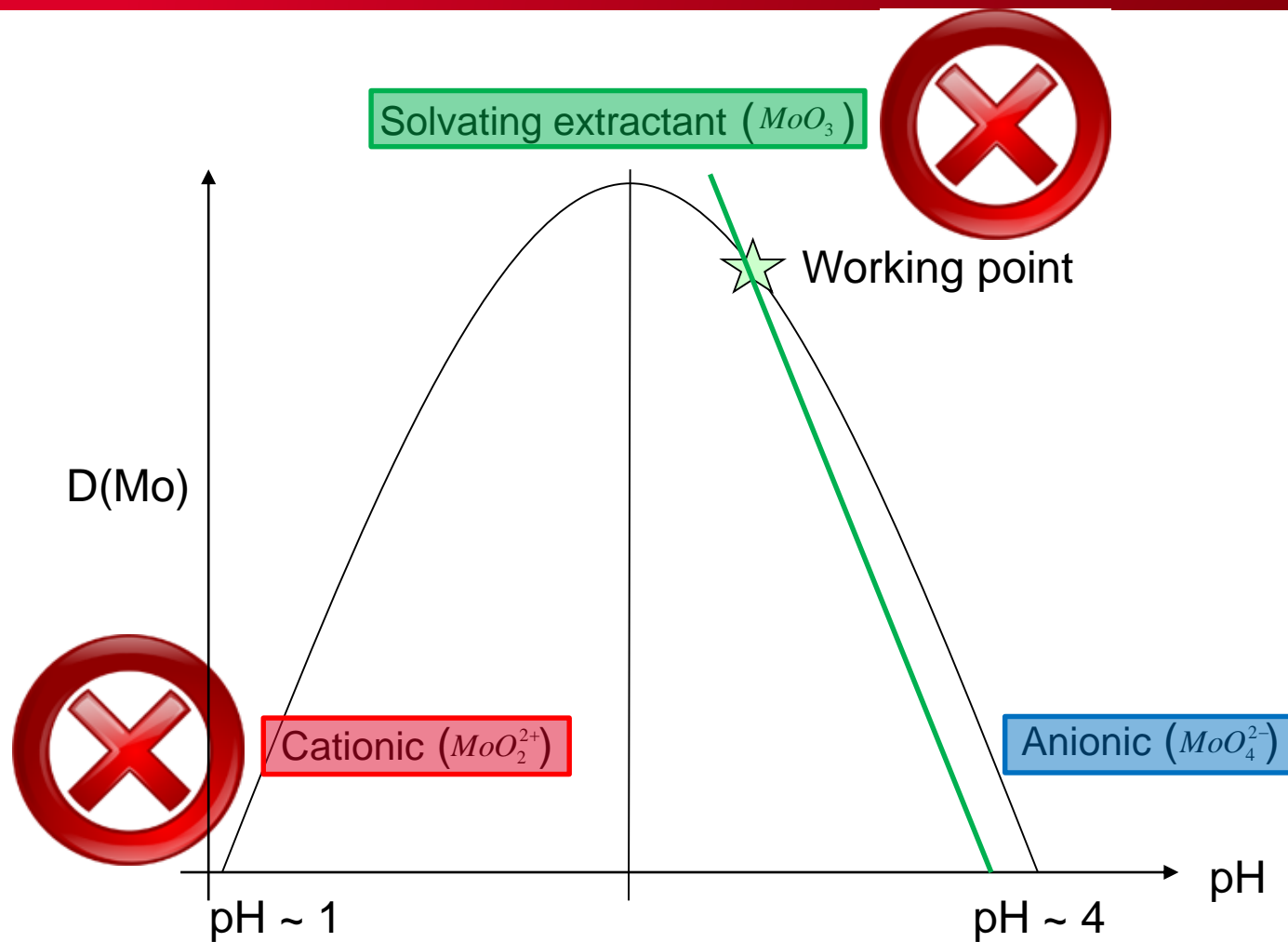
Chemical reaction	Formula	Log(K)
$MoO_2^{2+} / MoO_3$	$[MoO_2^{2+}] = K(MoO_2^{2+} / MoO_3) \times [MoO_3] \times [H^+]^2$	1.9
$MoO_3 / MoO_4^{2-}$	$[MoO_3] = K(MoO_3 / MoO_4^{2-}) \times [MoO_4^{2-}] \times [H^+]^2$	8.1
Cation exchanger	$\frac{[MoO_2 DEHP_2 HDEHP_2]}{[H^+]^2} = K_{ac} \times \frac{[MoO_2^{2+}]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

# Modelling of Mo(VI) behavior

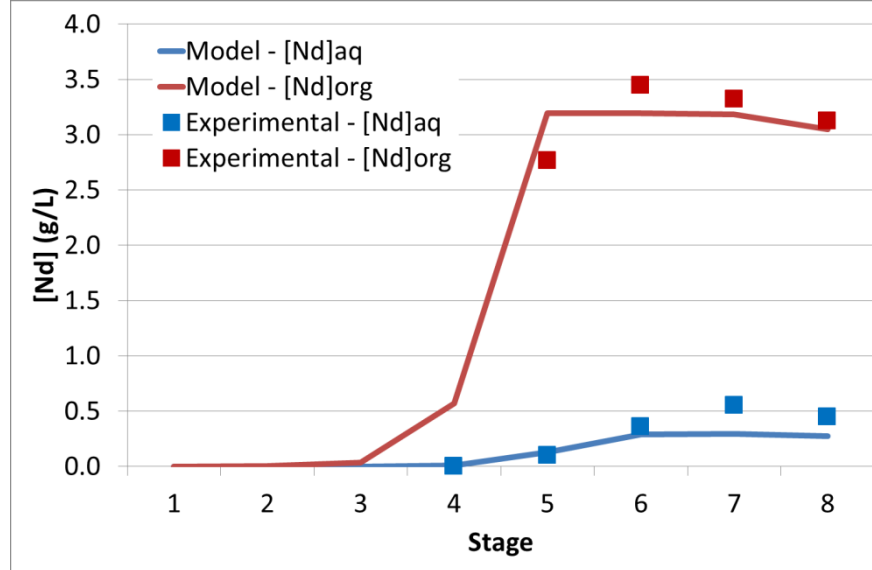
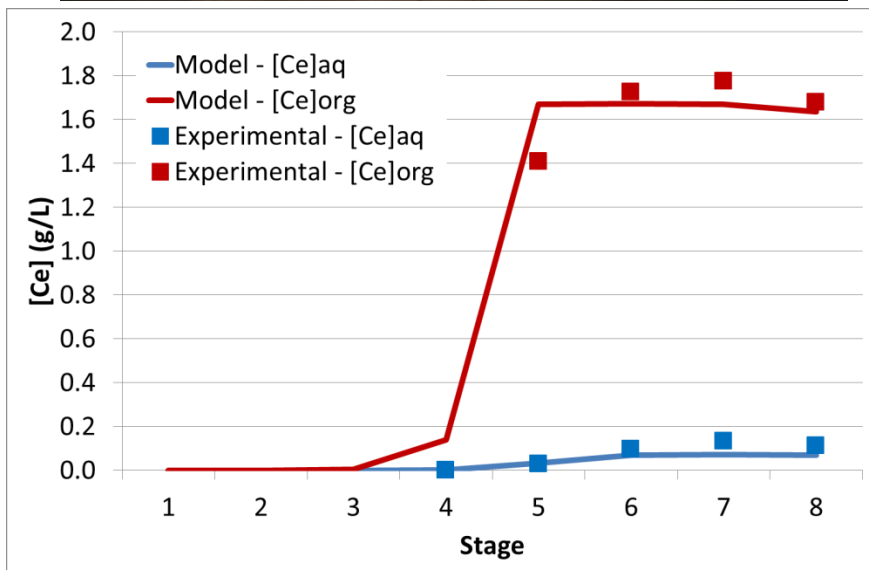
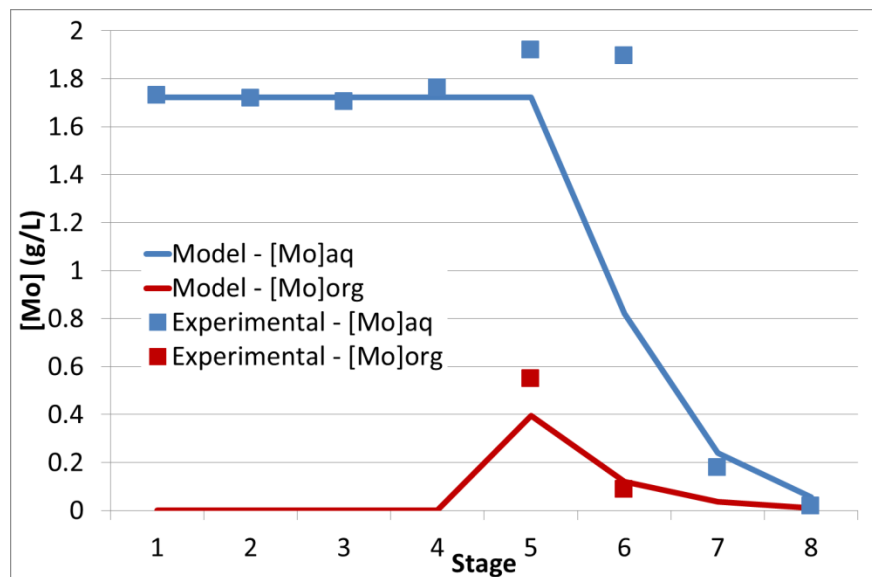


Model seems to be representative of Mo behavior

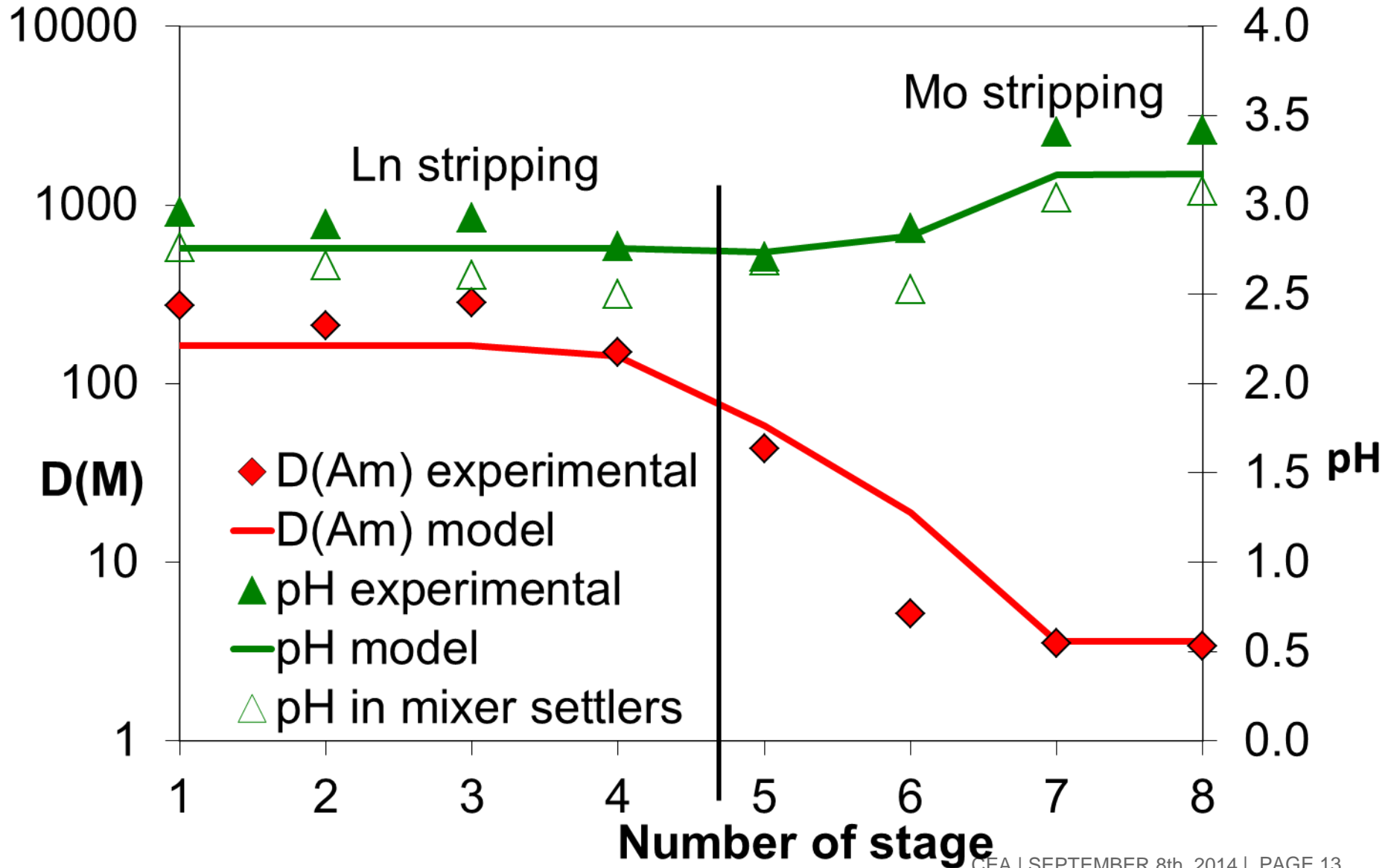
# Implementation in the PAREX code



## 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!



Commissariat à l'énergie atomique et aux énergies alternatives  
Centre de Marcoule | BP17171 | 30207 Bagnols-sur-Cèze Cedex  
T. +33 (0)4 66 79 77 00 | F. +33 (0)4 66 79 63 25

Etablissement public à caractère industriel et commercial | RCS Paris B 775 685 019

Direction de l'énergie nucléaire  
Département de radiochimie des procédés  
Service de modélisation et de chimie des  
procédés de séparation  
Laboratoire de modélisation des procédés de  
recyclage