



Horizon 2020
Programme

GENIORS

Research and Innovation Action (RIA)

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<http://geniors.eu/>



report on travel bursary and secondment grant attribution

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Summary

Final report on travel bursaries

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D12.1 Report on travel bursary and secondment grants

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Work Package 12: Training and Education

ULEEDS

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Work contribution to the following Domains and Work-Packages

- | | | | |
|--|------------------------------|-------------------------------|------------------------------|
| ☐ DOMAIN 1
WP1 | ☐ WP2 | ☐ WP3 | ☐ WP4 |
| ☐ DOMAIN 2
WP5 | ☐ WP6 | ☐ WP7 | |
| ☐ DOMAIN 3
WP8 | ☐ WP9 | ☐ WP10 | |
| DOMAIN 4 | | | |

☐ WP11 X WP12 ☐ WP13

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INTRODUCTION

The GENIORS project was awarded €20,000 to establish a travel fund to enable early career researchers connected to GENIORS to either (i) spend time on secondment working in other GENIORS Partner's facilities to enhance their research or (ii) attend selected dissemination & training events.

ADMINISTRATION OF THE FUND

An open call ran throughout the duration of the GENIORS project. Early career researchers seeking funding were invited to complete an application form (Appendix 1) for the proposed activity which was subsequently reviewed by members of the Executive Committee.

Successful applicants were required to submit a short report on their secondment/meeting/training event once complete. See Appendix 2 for the report template.

ALLOCATION OF FUNDING

A total of 10 awards were made – 6 secondments and 4 travel bursaries – the allocation of which is shown in the table below. Unfortunately owing to the Covid-19 pandemic some of the researchers were unable to complete their secondments. Reports from completed projects may be found in Appendix 1.

Name	Institution	Project	Type	Place	Amount awarded
Ivan Sanchez Garcia	CIEMAT	Gas generation in TODGA-DMDOHEMA/AHA-SO ₃ PhBTP systems	Secondment	NNL	€ 2,500
Magdalena Rejnis-Strzelak	Institute of Nuclear Chemistry and Technology, Warsaw	TRLFS investigations on the Cm ³⁺ and Eu ³⁺ complexes with an SO ₃ -Ph-BTP ⁴⁻ ligand in aqueous HNO ₃ solutions	Secondment	KIT-INE	€ 1,780
Annalisa Ossola	Politecnico di Milano	Investigation on loading capability and speciation of PyTri-Diol under process conditions	Secondment	CEA	€ 2,500
Daniel Theobald	University of Leeds	Computational Engineering for Nuclear Solvent Extraction Equipment	Travel bursary	Waste Management 2018, Phoenix, Arizona	€ 1,000
Thea Lyseid Authen	Chalmers University	Process development of the Chalmers Ganex process	Travel bursary	Fifteenth NEA IEMPT, Manchester, UK	€ 982
Thea Lyseid Authen	Chalmers University	Process development of the Chalmers Ganex process	Secondment	Forschungszentrum Jülich	€ 1,780
Nigel Lucas	Edinburgh University	The Electrochemical Removal of Neutron Poisons from molten salts for applications in Gen IV nuclear reactors and nuclear waste recycling	Travel Bursary	Processes: Flow-sheets & Simulation Workshop, Milan, Nov 4-6 2019	€ 750
Thea Lyseid Authen	Chalmers University	Process development of the Chalmers Ganex process	Secondment	Forschungszentrum Jülich	€ 1,533

Name	Institution	Project	Type	Place	Amount awarded
Maria Gallo	Universita di Parma		Secondment	CEA	€ 2,500
Alex Fells	University of Leeds	Experimental validation of a computational fluid dynamics model of a pulsed sieve-plate extraction column.	Travel bursary	CEA	€ 865

APPENDIX 1 TRAVEL FUND APPLICATION FORM

GENIORS Travel bursary and secondment grant scheme – call for proposals

The GENIORS consortium has been awarded funds to provide a limited number of travel bursaries and secondment grants for early career researchers.

A travel bursary (typically €1000) will go towards the cost of attending selected dissemination & training events (Please note that bursaries are not available for attendance at GENIORS yearly and half-yearly meetings).

A secondment grant (up to a maximum of €2500) will support a researcher connected to the GENIORS programme to spend up to two months working in other GENIORS partner's facilities to enhance their research.

Each successful applicant is required to provide a feedback report for inclusion in the final project report.

Scope of the call

The aim of the call is to provide travel bursaries / grants to enable early career researchers to attend events / undertake secondments that will enhance their research.

Eligibility

The call is open to all early career researchers connected to the GENIORS programme (less than three years in the organisation for the early career).

A maximum of 2 grants per Partner per event will be awarded.

How to apply

All applications must be made using the proposal template and signed by the researcher and their project supervisor. For secondment, the signature of the supervisor at the hosting facility is also mandatory.

Completed applications should be submitted via email to Lois S. Tovey (l.tovey@leeds.ac.uk) and Bruce Hanson (b.c.hanson@leeds.ac.uk).

The selection process

All applications received will be reviewed by the DM4 Leader, Bruce Hanson for eligibility and then applications will be approved by the Executive Committee.

Announcements

Successful applications will be notified via email which will include the procedure to claim the approved expenditure and the project feedback report template.

GENIORS Travel bursary and secondment grant scheme – application for funding

Researcher Name

Project Title

Supervisor Name and signature

For secondment, supervisor at hosting facility name and signature

Institution

Project Description

Please provide a description of your research project and justify your case for support. This should include:

- (i) For travel bursaries: How the event relates to your research and the specific learning outcomes envisaged;
- (ii) For secondment grants: How the secondment is connected to your research and the expected researcher outcomes, e.g. publications, etc...

Breakdown of costs

		€
Air Fares		
Rail Fares		
Accommodation		
Meals		
Conference fees		
Other expenses		

APPENDIX 2 TRAVEL FUND REPORT FORM

GENIORS Travel bursary and secondment grant scheme – Feedback report

Researcher Name

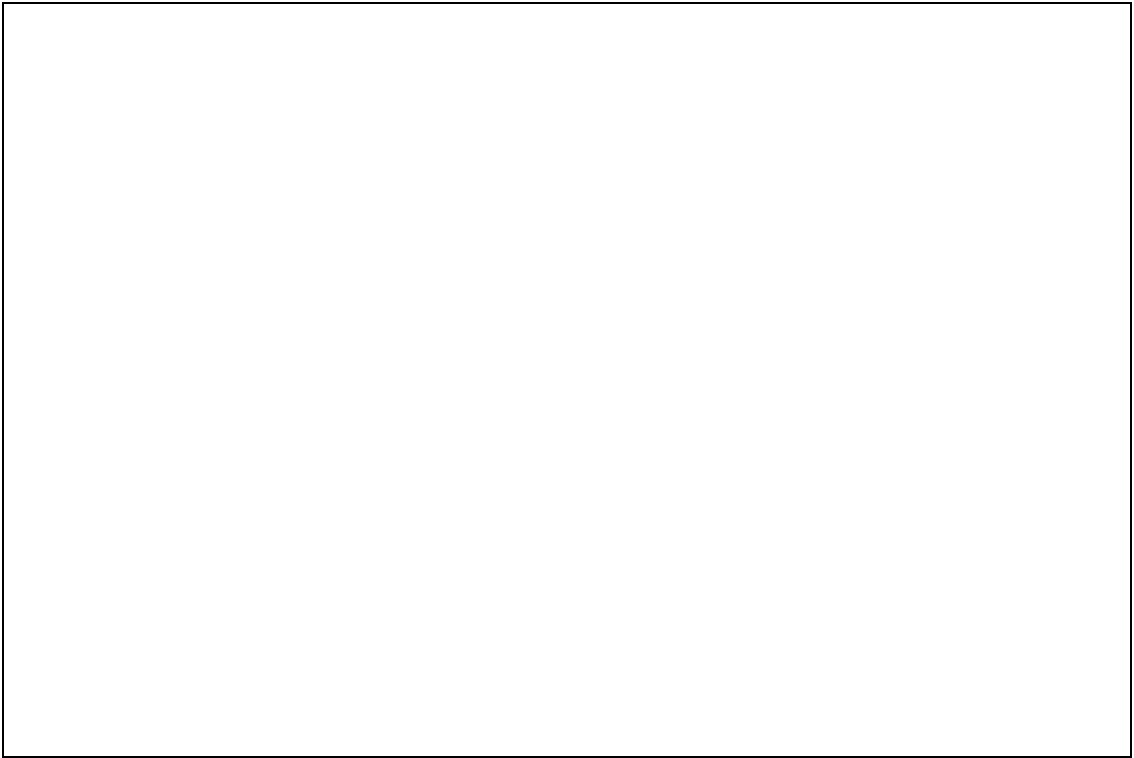
Project Title

Title of Conference/Place of Secondment (including dates)

Impact

Travel bursary - Please describe the conference/meeting attended and how you/your research benefitted from your attendance

Secondment - Please describe how the secondment has contributed to the advancement of your research and any outcomes e.g. publications, etc



APPENDIX 3 TRAVEL FUND REPORTS

GENIORS Travel bursary and secondment grant scheme – Feedback report

Researcher Name

Annalisa Ossola

Project Title

Investigation on loading capability of PyTri-Diol under process conditions

Title of Conference/Place of Secondment (including dates)

CEA - Commissariat à l'énergie atomique et aux énergies alternatives (Marcoule)
From 26/02/2019 to 27/04/2019

Impact

Travel bursary - Please describe the conference/meeting attended and how you/your research benefitted from your attendance

Secondment - Please describe how the secondment has contributed to the advancement of your research and any outcomes e.g. publications, etc

The aim of this project was the study of PyTri-Diol behavior in experimental conditions closer to the process ones. In fact, up to now, its stripping performances have been assessed only with aqueous solutions with TRansUranium elements (TRU) in trace amounts. Actually, the streams involved in a potential TRU/Lanthanides separation process would act on solutions with a higher content of TRU elements. In view of its future implementation in hydrometallurgical processes, the assessment of its loading capability is a key requirement.

Thanks to this project, both $^{241}\text{Am(III)}$ and $^{239}\text{Pu(IV)}$ loading capabilities of PyTriDiol were successfully proved, leading to the first demonstration of PyTri-Diol applicability to both *i*-SANEX and EURO-GANEX processes. In particular, stripping tests were carried out with organic phases loaded with 1 mM of trivalent Am (*i*-SANEX process applicability) and 15 mM of tetravalent Pu (EURO-GANEX process applicability), besides trivalent Eu as radiotracer and 20 mM of Y and stable Lns (not measured). In the case of *i*-SANEX process, PyTri-Diol loading capability was ascertained also with aged and irradiated stripping phases.

Furthermore, the results concerning Pu(IV) loading capability were so promising that the system composed of PyTri-Diol + AHA + TODGA and DMDOHEMA was selected as new EURO-GANEX reference system by the European scientific community of Horizon 2020 GENIORS project.

Tests description, working conditions and results achieved will be published soon.

Up to now, no presentations at conferences are planned.

GENIORS Travel bursary and secondment grant scheme – Feedback report

Researcher Name

Daniel Wesley Theobald

Project Title

Computational Nuclear Engineering for Solvent Extraction Processes

Title of Conference/Place of Secondment (including dates)

WM2018 Conference, March 18-22 2018, Phoenix, Arizona, USA

IMPACT

Travel bursary - Please describe the conference/meeting attended and how you/your research benefitted from your attendance

Secondment - Please describe how the secondment has contributed to the

I was given the opportunity disseminated my research through a 20 minute presentation on the Wednesday of the conference and through publication of a subsequent conference proceedings paper:

<http://eprints.whiterose.ac.uk/134953/>.

The publication released here contribute to my final PhD thesis included as part of the total package of work to be assessed.

The Oral presentation was made during the 'high-Level waste, spent nuclear fuel' panel within the 'advancements in HLW separations and reprocessing session' organised by those from ORNL (USA) talking alongside CEA Marcoule and AREVA. My audience was those interested in developments in Gen IV fuel reprocessing, largely comprised of experts from international and the American legacy reprocessing/research facilities.

Additionally, I was able to network with international researchers within my field particularly with those from CEA (France) and Orano (France/USA). A UK consultant engineer approached me with interest in collaborating on analysis of an Ion exchange column using ULeeds expertise in computational fluid dynamics.

I also attended talks on computational modelling from Savanna River Remediation, Idaho National lab, and Los Alamos, as well as reprocessing talks from Argonne National Lab and speakers within my own panel session.

advancement of your research and any outcomes e.g. publications, etc

N/A

GENIORS Travel bursary and secondment grant scheme – Feedback report

Researcher Name

Thea Lyseid Authen

Project Title

Process development of the Chalmers Ganex process

TITLE OF CONFERENCE/PLACE OF SECONDMENT (INCLUDING DATES)

Fifteenth NEA Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation (15IEMPT)

And

International Nuclear Engineering Conference 2018

IMPACT

Travel bursary - Please describe the conference/meeting attended and how you/your research benefitted from your attendance

Secondment - Please describe how the secondment has contributed to the advancement of your research and any outcomes e.g. publications, etc

'This grant was initially awarded to attend the Fifteenth NEA Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation (15IEMPT) in Manchester in Sep/Oct 2018. However, by cutting costs on accommodation and flights, the grant was sufficient to also cover my attendance at the International Nuclear Engineering Conference, also in Manchester 4th-5th October 2018.

15IEMPT

At this conference, I listened to numerous presentations of high relevance to my research field and specific project. Of particular interest were session 1,2 and 6 of the conference, covering the topics of international and national P&T programs, fuel cycle strategies and advanced nuclear fuel cycle. The latter session proved to be the most relevant to my own research. It was indeed very interesting to not only learn of the other approaches to partitioning of minor actinides in other countries, outside the EU, but also to compare work methods with other institutions. I co-chaired this session, which gave me good practice in critical thinking in order to prepare questions for the discussion afterwards. Of most value to my development as a researcher, was the poster session, however. Being the first poster session where I presented my own poster and research, it was very educational and constructive to receive critical questions, comments and suggestions for further work. I got to discuss the use of FS-13 as a diluent with some of the Russian attendees, which have long experience with this particular diluent, which I found very valuable. In conclusion, I found the 15IEMPT to be very enjoyable, educational and a great setting for networking with fellow researchers within the field of partitioning and transmutation.

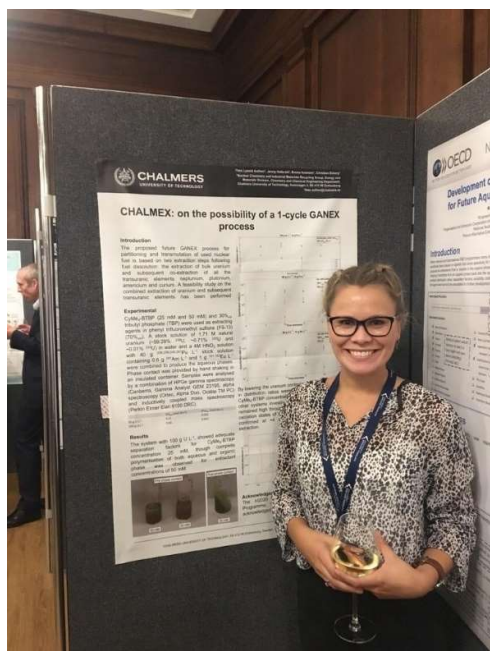


Figure 1: Poster presentation at 15IEMPT

International Nuclear Engineering Conference

The International Nuclear Engineering Conference, hosted by the Institution of Chemical Engineers, in Manchester 2018, was a conference with a heavy presence of industrial institutions and research institutions alike. Of relevance to my research project, it covered the topics of nuclear waste management and spent fuel and nuclear material management. It was very inspiring to hear the industrial approach to research, and to see research actually being employed in industry and improving industrial processes. The presentations presented a view different from those presented when at pure academic conferences: It had a focus of real life application, and I found it very encouraging to see that there are companies wanting to employ the technology I work with, not even in the too distant future. In academia the timeplan is somewhat diffuse, the terminology used is “In the future” or “in 50 years”, while the industry in general says “we want this yesterday”.

Another benefit of this conference was to be able to network, and discuss my work with engineers. Having a background in engineering myself makes such conversations highly valuable, as I was able to discuss more process-related topics (compared to pure chemistry related topics). Engineers deal with processes on a larger scale, which is the ultimate (personal) aim of my PhD project: to increase TRL by proving the CHALMEX on a larger scale. I got advice on how to start working with this, and which priorities to make from discussions at this conference.

GENIORS Travel bursary and secondment grant scheme – Feedback report

Researcher Name

Nigel Lucas

Project Title

Development of Electrochemical Sensors for Nuclear Waste Recycling Methods

Title of Conference/Place of Secondment (including dates)

Geniors workshop “process flow sheets & simulation” in Milan

IMPACT

Travel bursary - Please describe the conference/meeting attended and how you/your research benefitted from your attendance

Secondment - Please describe how the secondment has contributed to the advancement of your research and any outcomes e.g. publications, etc

I attended the workshop at Milan University, where there was a workshop for developing a flow sheet for Euro Ganex.

The trip highlighted some key applications area where our electrochemical sensors could be used. As currently lots of the applications are in pyrochemical reprocessing. Networked with lots of useful people who will be hugely useful for upcoming research. I also learned a great deal about the current state of nuclear applications globally which will have an effect on the direction of my research.

GENIORS Travel bursary and secondment grant scheme – Feedback report

Researcher Name

Thea Lyseid Authen

Project Title

Process development of Chalmex Process

Title of Conference/Place of Secondment (including dates)

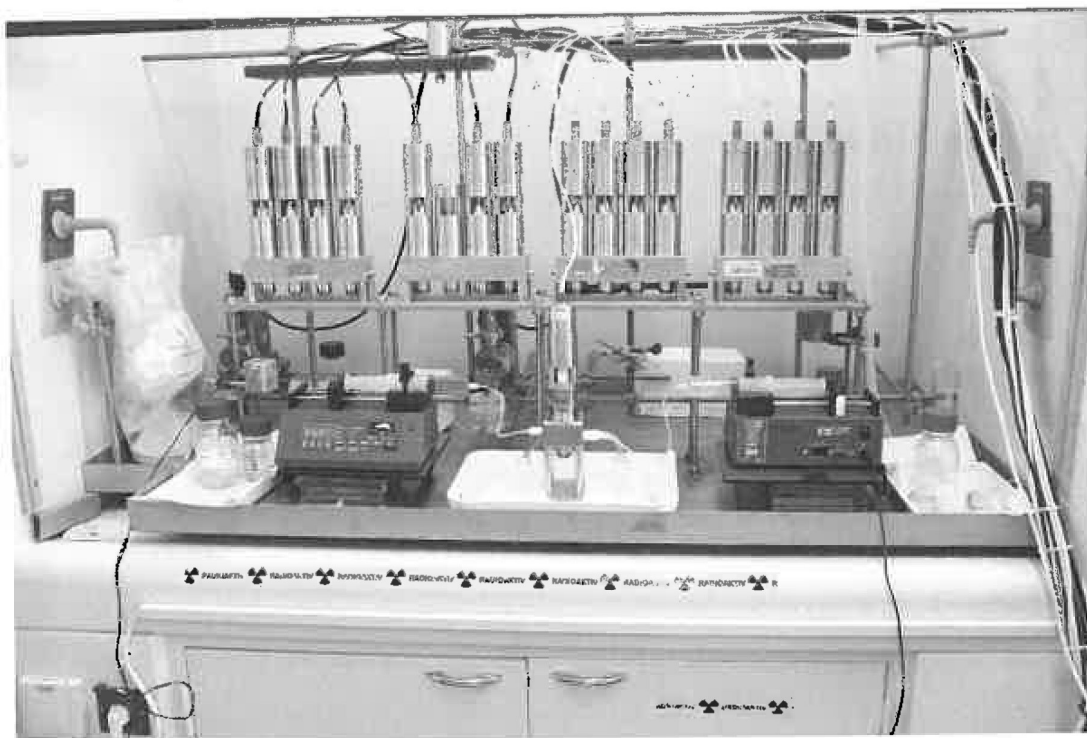
Jülich Forschungszentrum, Germany

Impact

Travel bursary - Please describe the conference/meeting attended and how you/your research benefitted from your attendance

Secondment - Please describe how the secondment has contributed to the advancement of your research and any outcomes e.g. publications, etc

Over a period of 18 days in March 2019 I completed a research secondment at Jülich Forschungszentrum in Germany, hosted by Giuseppe Modolo and Andreas Wilden. The initial aim of the visit was to test the CHALMEX solvent's suitability in a centrifugal contactor, and to determine the performance of the solvent on simulated highly active raffinate. During the course of the secondment I also did complimentary experiments. These experiments included acid extraction experiments, kinetics of fission product extraction, large scale batch extraction experiments with scrubbing and stripping steps.



Not only did I produce a lot of experimental result, providing enough data for at least 2 manuscripts which will be submitted to scientific journals, I have also learned a great deal regarding experimental procedures and data processing. I learned how to work cleaner and more efficient when dealing with radioactive tracers, and I have since returning to Gothenburg used these techniques in my lab. I was also lucky enough to get to know a lot of highly skilled scientists whom provided insightful advice and discussions, further increasing my professional network. Despite the results from the experiments not being the most promising, I would conclude that it was a successful stay scientifically. Since the stay, I have gained a focus my research was lacking before, and I feel more confident in my upcoming licentiate thesis and defence.

GENIORS Travel bursary and secondment grant scheme – Feedback report

Researcher Name

Thea Lyseid Authen

Project Title

Process development of Chalmex Process

Title of Conference/Place of Secondment (including dates)

Jülich Forschungszentrum, Germany

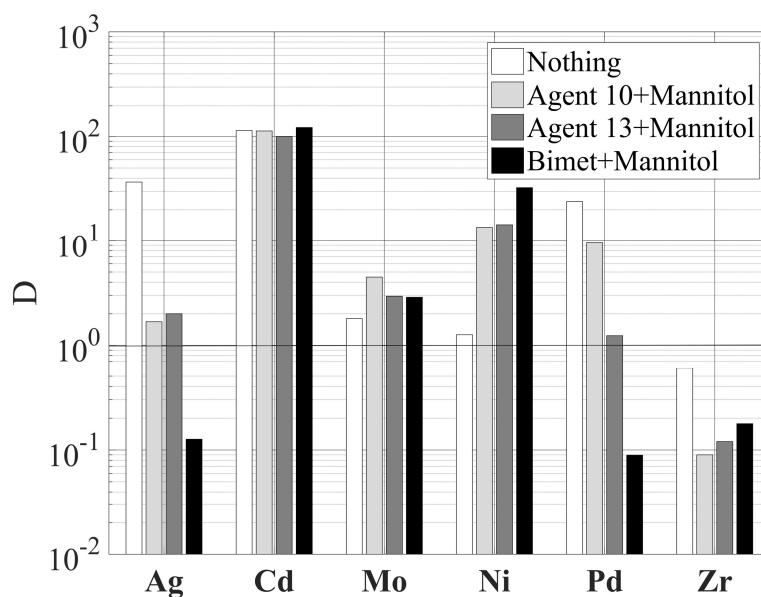
IMPACT

Travel bursary - Please describe the conference/meeting attended and how you/your research benefitted from your attendance

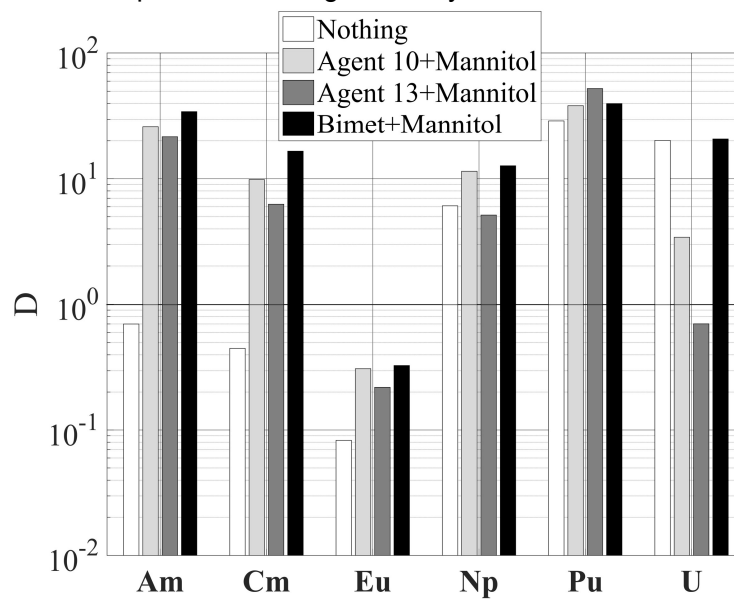
Secondment - Please describe how the secondment has contributed to the advancement of your research and any outcomes e.g. publications, etc

Over one month, lasting from the end of November to the end of December 2019, I completed a second research stay with Jülich Forschungszentrum. My hosts were Prof. Giuseppe Modolo and Dr. Andreas Wilden. The purpose of the stay was to continue the development and testing of the CHALMEX process under more process-like conditions. Jülich forschungszentrum have both the expertise and unique facilities to accommodate such experiments.

Since the last visit in March 2019, efforts had been focused on fission product complexing agents. These most promising agents were now tested using simulated PUREX raffinate to determine their effectiveness in the presence of a highly complex simulated spent fuel solution. Novel extracting agents (agent 10 and agent 13) were also tested for reference.

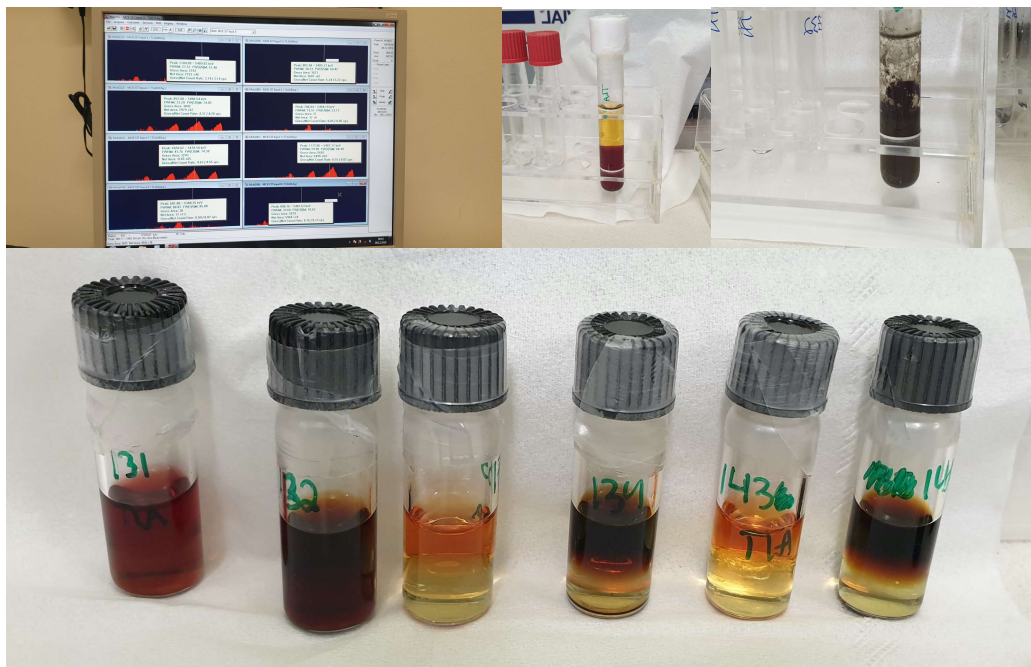


Overall, the performance of bimet combined with mannitol was the most promising when considering the fission product masking efficiency and the extraction of actinides



in their presence.

Other preparatory experiments for flowsheet tests were also conducted, including establishing the acid dependency of actinide and fission product extraction using trace metal concentrations, in the presence and absence of masking agents. Based on these results two flowsheet tests were conducted, the second with improvements of the first. In the final flowsheet test, good results were achieved for the extraction and separation of actinides.



Overall, the stay at Jülich Forschungszentrum was highly educational and productive. I am convinced that the support and guidance of Prof. Modolo and Dr. Wilden provided me with during my two stays enabled me to successfully write and defend my licentiate thesis. All the produced results contributed to a major extent to my licentiate thesis and defence (equivalent to transfer viva: "CHALMEX FS-13 investigations for process implementation"- Authen, 2020). The secondment has so far also led to one successful publication in Solvent Extraction and Ion Exchange ("Batch Flowsheet Test for a GANEX-type Process: The CHALMEX Process": accepted with minor revision). Part of the experimental work has been included in a second manuscript being prepared for submission later this year.

Report GENIORS

Researcher: Maria Chiara Gullo

Project Title: Exploiting the DGA binding group to improve performance of lipophilic lanthanide extractants

Supervisor: Alessandro Casnati

Supervisor at hosting facility: Wim Verboom

Institution: University of Twente (UTwente)

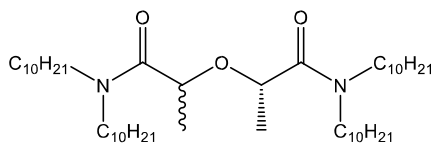
Period: 15th September 2020 – 15th December 2020

Introduction:

DGAs (diglycolamides) are considered an important class of extractants for actinide partitioning. Within the GENIORS program there is a growing interest in the exploitation of DGA chelating unit in order to extract Ln ions in the organic phase. The efficiency and selectivity of DGA based ligands depends on the alkyl chains present on the amide-N atom and on the presence of additional alkyl chains inserted in the alpha position of the carboxy group (O-CHRC=O). Surprisingly also the stereochemistry of the molecule affects the properties of the ligands. Indeed, the *cis*-mTODGA was found to be much more efficient than the racemic mixture of its diastereomers besides it showed a better selectivity for Ln (III) over Am (III) and Cm (III).¹ Furthermore the tetradecyl derivative (*cis*mTDDGA) is getting more and more attention in the GENIORS program.² The secondment of Maria Chiara is aiming to synthesize a few novel ligands showing different structural modifications which might improve the extraction properties of the ligands.

Work:

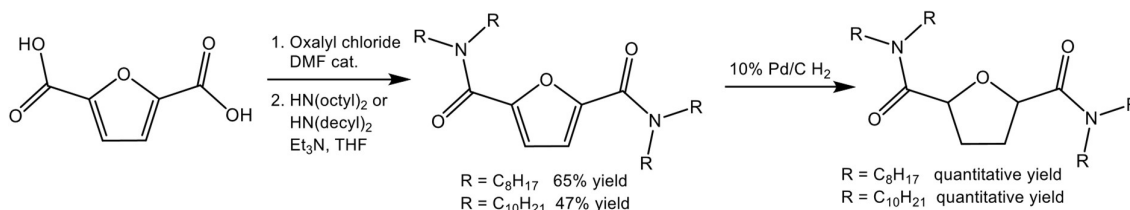
The work mainly focused on the preparation of ligands related to mTDDGA.



cis- and *trans*-diastereomer of mTDDGA

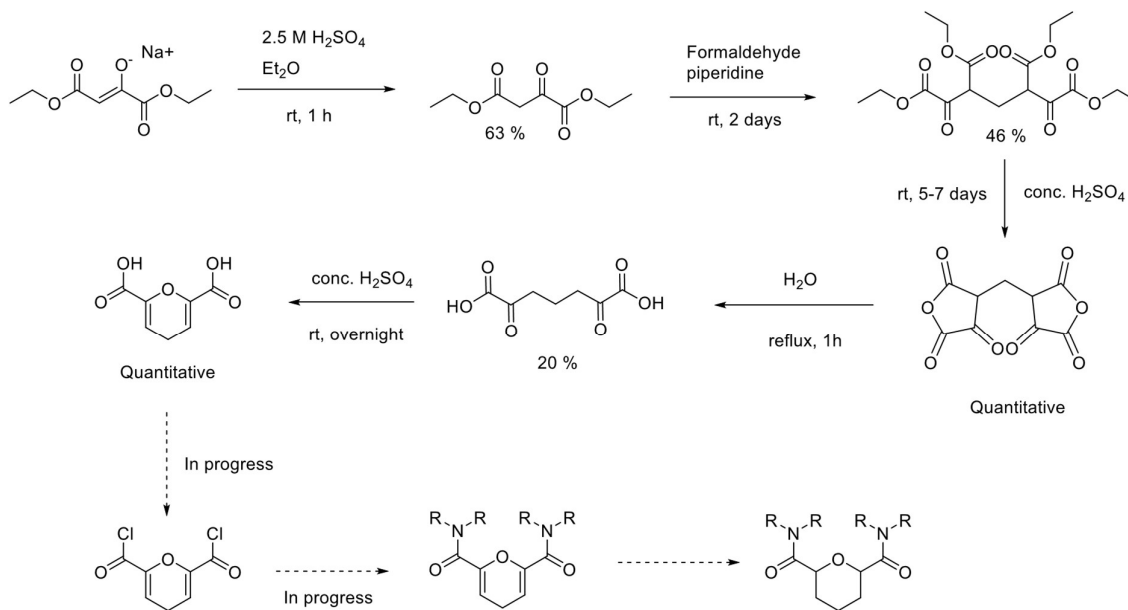
The results obtained from the studies on m-TDDGA demonstrated how the stereochemistry influenced ligands properties. Therefore, the effect of rigidification of the ligand structure maintaining the *cis*-disposition of the alpha substituents has been studied.

Commercially available furan 2,5-dicarboxylic acid was converted into the corresponding dichloride. The intermediate was immediately reacted with the desired amine to give the corresponding diamide derivative. Subsequent reduction with H₂ using Pd/C as a catalyst afforded the target ligands (both with C8 and C10 chains), Scheme 1.



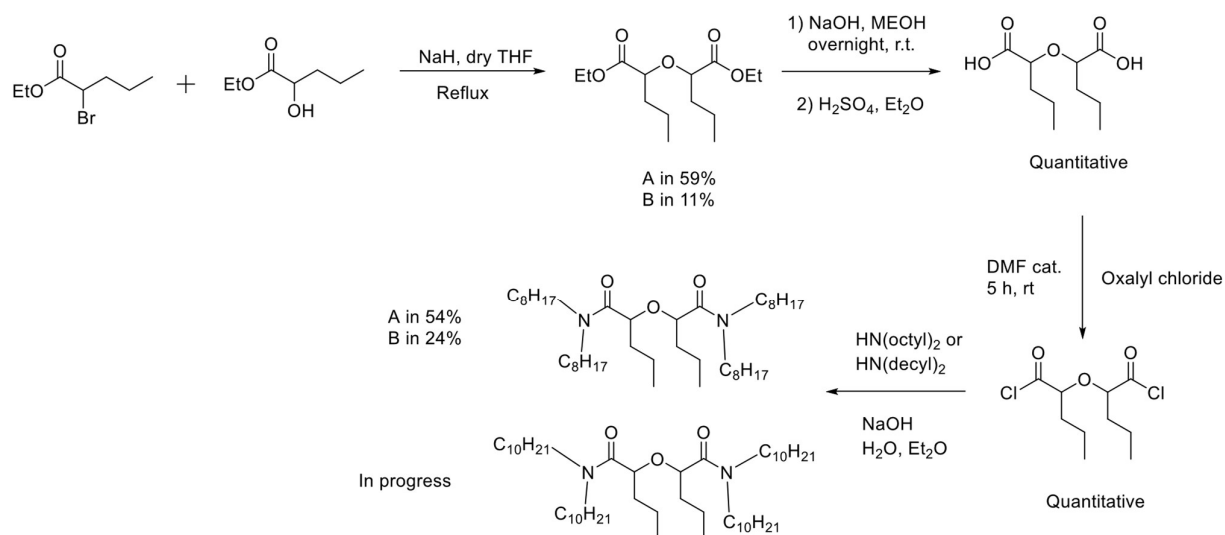
Scheme 1

The preparation of the corresponding ligands with a six-membered ring is in progress, Scheme 2. For this purpose 4H-pyran-2,6-dicarboxylic acid has to be prepared via a multistep procedure³.



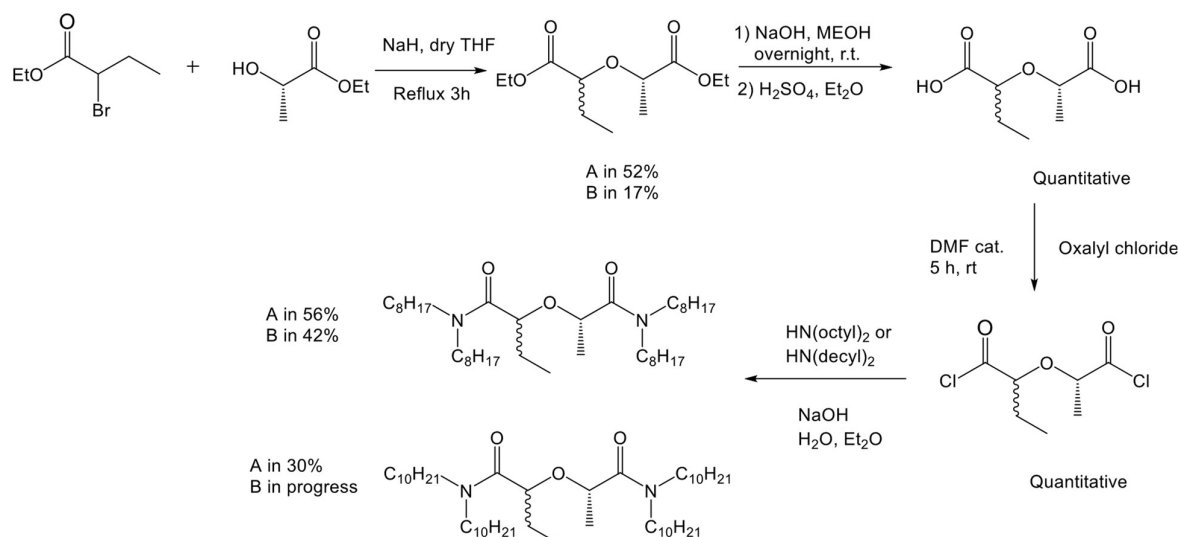
Scheme 2

A further modification involved replacing the methyl groups in the backbone of mTDDGA by propyl groups. The synthesis was performed in the same way as described for mTDDGA, now starting from ethyl 2-bromopentanoate and ethyl 2-hydroxypentanoate, Scheme 3. The diastereomers (A and B) were separated in the diester stage.



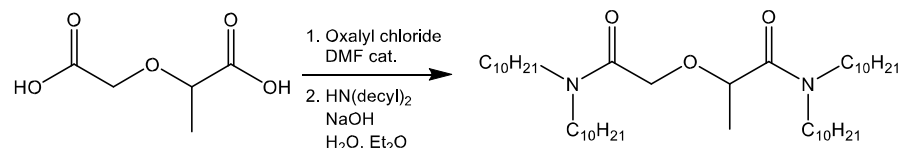
Scheme 3

To further evaluate the effect of substituent we thought to synthesize a derivative with asymmetrical substituents at the backbone. The synthesis proceeds as so far described, however, now starting from ethyl 2-bromobutanoate and (S)-ethyl lactate, Scheme 4.



Scheme 4

On request of Juelich a sample of the C10 derivative of TWE-21 (C10-TWE-21) was prepared as outlined in Scheme 5. The yield has to be optimized.



C10-TWE-21 Conclusions:

During this research activity it was possible to synthesize two different DGA based new ligands wearing additional alkyl chains in the alpha position of the carboxy group (O-CHRC=O). In particular a symmetric derivative presenting two propyl chains at the backbone (p-TODGA) and one asymmetric derivative presenting a methyl and a ethyl chain (e,m-TODGA). The corresponding ligands presenting C10 chains on the amide-N atom are in progress.

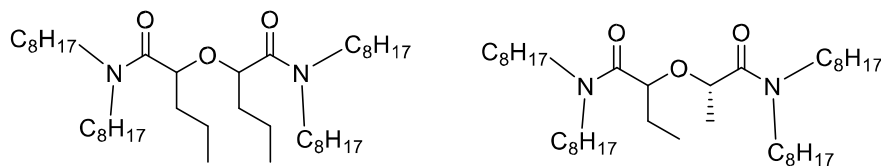
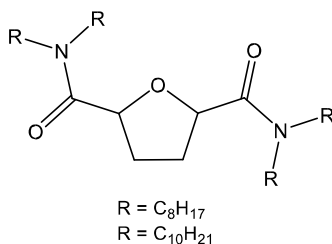


Figure 1. Structure of p-TODGA (left) and e,m-TODGA (right)

In order to evaluate the effect of rigidification of the ligand structure, a derivative with a five-membered ring was synthesized with both C8 and C10 chains.



The work has successfully been done within a period of two months and presents the basis for a profitable joint publication.

References

- (1) Wilden, A.; Kowalski, P. M.; Klač, L.; Kraus, B.; Kreft, F.; Modolo, G.; Li, Y.; Rothe, J.; Dardenne, K.; Geist, A.; Leoncini, A.; Huskens, J.; Verboom, W. Unprecedented Inversion of Selectivity and Extraordinary Difference in the Complexation of Trivalent f Elements by Diastereomers of a Methylated Diglycolamide. *Chem. - A Eur. J.* **2019**, 25 (21), 5507–5513. <https://doi.org/10.1002/chem.201806161>.
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<https://doi.org/10.1007/s10967-017-5614-2>.
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