



Noordwijk, 08 April 2009

Dr. V. Van Speybroeck
University Gent
Center for Molecular Modelling
Proeftuinstraat 86
B-9000 Gent, Belgium

Exchange of Letters - PRODEX Experiment Arrangement.

Dear Madam,

With reference to the Institute Agreement signed by ESA on 21 October 1996 and by the Institute on 04 November 1996 we hereby send you the conditions of the PRODEX Experiment Arrangement between ESA and your Institute:

UG
Phone: +32 9 264 65 59
Fax: +32 9 264 65 60
Email: Veronique.Van Speybroeck@UGent.be

related to C90364 "Ordered Liquid Phases - OLP's". The ESA representative for all administrative and contractual matters is Mrs V. Dowson, and for all technical/scientific matters it is Mr. O. Minster.

The total price of the present arrangement amounts to 57,750 €, and upon your signature of the present letter an advance payment of 25% of the total limit of liability can be invoiced to ESA. Please note that this advance payment will have to be set off against any future claims for reimbursement of costs. Furthermore, all invoices should mention the European standard "IBAN" and "BIC" as bank account identifiers; failing to do so will block the settlement of the payment.

The term of the project shall be the time period 01 January 2009 through 31 December 2010.

I would appreciate if you could sign and approve the present letters and return one original to me at your earliest convenience.

I am looking forward to a fruitful co-operation,

Sincerely Yours,

H. Schroeven-Deceuninck
Head of the PRODEX Office

Received, accepted and signed by Institute:

Place / date:

.....
V. Van Speybroeck 28/4/09

PRODEX EXPERIMENT ARRANGEMENT

ARTICLE 1: DEFINITIONS - PURPOSE OF THE ARRANGEMENT - APPENDICES

1. Throughout the present Arrangement the terms laid down in the left column below shall have the meaning set out opposite:

"Funds": An amount of money whose maximum is laid down in Article 2;

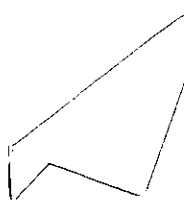
"Project": Institute's project specified in Appendix 1, certified by the Agency's PRODEX Office as
- eligible for financial support according to the Financial Plan (Appendix 2) approved by the relevant Participating State,

"Cost": Allowable cost of these categories:
- labour cost
- operational cost in the sense defined in Appendix 2
- travel expenses
-
incurred by the Institute in execution of the Project.

2. By entering into the PRODEX Experiment Arrangement the Agency undertakes to reimburse the Institute certain cost incurred in execution of the Project. Purpose of this arrangement is the detailed implementation of said undertaking.

An obligation on the part of the Institute to carry out the Project is not created by this arrangement. Any other arrangement or agreement by which the Institute undertakes to carry out the Project remains unaffected by the present arrangement, save that the Agency acquires hereunder the rights to access, to audit, and certain licenses in intellectual property rights; details are stipulated in Article 4 and Appendix 4.

3. The Institute may claim the Funds subject to the provisions set forth in Articles 2 through 6 below.
4. The Institute shall utilise the Funds and any part thereof exclusively for defraying, in due time, the Cost incurred during the term of the Project defined in Article 3.1 below.
5. Appendix 1 (Work Description), Appendix 2 (Financial Plan) remain unaffected by this arrangement; Appendices 1 and 2 are appended for information only. Appendix 3 (Contract Change Notice procedure and form) and Appendix 4 (General Conditions) shall form an integral part of this arrangement.



ARTICLE 2: FUNDS

1. The Funds available for the present arrangement amount to(see cover letter)
2. The above amount is stated to be a limit of liability in the sense defined in Clause 9 of Annex I to the "General Conditions", attached as Appendix 4 hereto.
3. The above amount excludes profit for the Institute (not allowed) and value added tax on the costs charged to the Agency (so far as the Agency is exempted from VAT applied by the Agency's Member States).
4. (Optional)
The above amount is broken down into subtotals per cost category and/or per year as specified in Appendix 2 hereto.

ARTICLE 3: TERM OF THE PROJECT

1. Term of the Project shall be the time period stated in the cover letter.
2. Cost incurred outside said term shall not entitle the Institute to any payment under this arrangement.

ARTICLE 4: OTHER CONDITIONS

"General Conditions" lay down in Appendix 4 shall apply, with the amendments or replacements set forth in the Articles of this arrangement. The applicable General Conditions shall be construed and interpreted with due regard to the specific nature of this arrangement and its Article 1.2 Sentence 3 in particular. The Institute shall be deemed the "Contractor" wherever mentioned in those General Conditions.

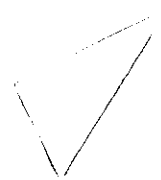
CLAUSE 2: APPROVAL

Offers and acceptances with regard to arrangements are not binding on the Agency unless approved in writing by its Director General or his authorised representative.

For the purpose of this arrangement the authorised representative of the Agency's Director General is:

Mrs. H. Schroeven-Deceuninck,
Head of the PRODEX Office.

She is authorised by the Agency to sign the present arrangement on its behalf.



CLAUSE 5: AGENCY'S REPRESENTATIVES - INSPECTIONS

The Agency shall have the right to check the performance of the Project, and for this purpose the Agency nominates its representatives identified in Clause 7 here below.

The Institute shall in this respect, and in accordance with any relevant security regulations, give the representatives of the Agency access to its premises and shall give all other necessary assistance in order that they may fulfil their task.

CLAUSE 7: COMMUNICATIONS

All correspondence for either party shall be sent to the address and the representative in charge identified herein below, with a copy to the other representative(s) where any mixed nature of the matter so requires:

For the Agency to:

ESTEC
P.O. Box 299
NL-2200 AG Noordwijk

For the Institute to:

See address, fax and phone number in the cover letter.

Tel/Fax: +31 71 56 + extension below

The Agency's representatives are:

- Mr. E. Zanuttini (RES-FET-Team 1) for invoices
(e-mail: Elmer.Zanuttini@esa.int; fax ext. 55186; phone ext. 56362)

and :

- Mrs. V. Dowson (SRE-MR) for all administrative and contractual matters
(e-mail: Veronique.Dowson@esa.int; fax ext. 54693; phone ext. 53243)
- Mr. O. Minster (HSF-USP) for all technical and scientific matters
(e-mail: Olivier.Minster@esa.int; fax ext. 53661; phone ext. 54764)

The Institute's representative(s) is (are) as stated in the cover letter.

CLAUSE 12 - APPLICABLE LAW

The arrangement shall be governed by the laws of the country of residence of the Institute.

CLAUSE 13 - ARBITRATION

The arbitration proceedings referred to in Clause 13 shall take place in the capital of country of the residence of the Institute.

CLAUSE 22 – INVOICES, PLACE AND CURRENCY OF PAYMENT

1. Payments shall be made by the Agency to the account specified by the Contractor. Such information shall clearly indicate the IBAN and BIC/SWIFT codes. Payments shall be considered as effected on time if the Agency's orders of payment reach its bank within the payment period stipulated in Clauses 20 & 21.

2. EFIS
 - 2.1. The Contractor undertakes to ensure that all invoices are submitted to the ESTEC Finance Division, Central Invoice Registration office (CIR) by electronic transmission, using the Agency's EFIS System. (<http://efis.esa.int>)
 - 2.2. The Contractor undertakes to submit complete invoices in adhering strictly to the instructions contained in the standard EFIS package, e.g. with regard to supporting documentation, information on billing of taxes and duties, etc.
 - 2.3. If the Agency's EFIS system is not operational with the Contractor, the Contractor may submit invoices in paper format in 5 copies, together with justifying documentation as required by the contract. All other non-EFIS specific provisions of this clause 22 shall however apply.
 - 2.4. As soon as EFIS is operational with the Contractor, this Clause 22 shall apply in its entirety to all contracts between the Contractor and the Agency.
 - 2.5. Any questions arising concerning the operation of EFIS shall be discussed between the Contractor and ESTEC Finance Division.

ARTICLE 5: PAYMENTS

1. Within the limits specified in Article 2 the Institute may claim in arrears payment of the Cost incurred. The Agency shall effect such payment after receipt of the respective invoice, which must identify the cost category/ies concerned and bear a statement by the Institute's financial controller that the invoiced costs are fair and reasonable, do not include profit and have been incurred exclusively in execution of the Project as defined in Article 1.1 and during the term specified in Article 3.1.

2. The Agency shall make an advance payment as stated in the cover letter, upon signature of the cover letter by both parties and against submission of an invoice. Any claims for reimbursement of Costs incurred shall be set off against such advance payment; payments in excess of the advance payment shall be effected only once the advance payment has been consumed in the aforesaid manner.

ARTICLE 6: CESSATION, REFUND OF PAYMENTS

1. Notwithstanding any other provision of this Arrangement, the Agency may:
 - 1.1 cease to effect any payments not already fallen due under this arrangement in case of unsatisfactory progress within the Project, provided the Participating State having approved Appendix 2 demands cessation of payments in writing;

- 1.2 cease to effect any payments in any of the following cases:
 - a situation as per Clause 34.1 lit. a) of the General Conditions occurs;
 - a situation as specified in Paragraph 2.2 below occurs.

- 2.1 The Agency may require the Institute to return to the Agency payments effected under this arrangement if and to the extent an audit carried out by the Agency or by the relevant national audit authority reveals any incorrectness of invoices or unauthorised use of Funds.

- 2.2 The Agency may require the Institute to return to the Agency all payments effected under this arrangement in case a situation as per Clause 34.1 lit. b) of the General Conditions occurs. Within said Clause the words "by deceit concerning the nature, quality or quantity of the supplies, and the methods or processes of manufacture employed" shall be deleted.

PRODEX Experiment Arrangement
Guideline for the preparation of its Appendices 1 (Work Description) and 2 (Financial Plan)

Part I: The Work Description. Appendix 1

1) Work Description:

The Work Description is to identify the Project, i.e. the work in execution of which reimbursable cost will be incurred by the Institute during the term of the Implementation Arrangement.

Length: One page should be sufficient but in no way be regarded as a firm limit.

2) Distinctions as to 'who' and 'when':

The work to be carried by the Institute and to be paid for by ESA under the Implementation PRODEX Experiment Arrangement (the Project) is to be clearly separated from the work to be carried out by others (if the latter is mentioned at all).

Project activities to be carried out during the term specified in the Implementation PRODEX Experiment Arrangement must be clearly separated from work outside said term (if the latter is mentioned at all).

3) Compatibility with other Applicable Documents:

Subject to 1)- 2) above the Work Description must correspond to the work description submitted to the relevant national authority in support of the Financial Plan, and is covered by the Institute Agreement.

Part II: The Financial Plan. Appendix 2 (see figure 1)

1) Content

The Financial Plan's minimum content will encompass:

- a) Title of the Project and identification of the Institute
- b) Cost categories such as:
 - Salaries (please specify employee(s) name(s))
 - Travel
 - Miscellaneous
- Overheads: Please note that for Belgium, overheads can only be charged for a **maximum of 5% on Salary costs.**
 - Equipment < 5000 Euros purchased directly by Institute/University
 - etc.
- c) Amounts.
Please note that all figures should be mentioned in Euro and that they should be exclusive of VAT in the Agency's Member States.
- d) Time periods

[Ideally this Appendix will be a copy of the document, which was approved by the Delegation.]

2) Procurement of equipment > 5000 Euro (not counting VAT)

This category should not be integrated in the Financial Plan below, but listed separately, seeing that the equipment may be available via PRODEX Office by means of placing a Purchase Order by the Agency (See figure 2). This way of doing would have the advantage of making sure that the equipment purchased for the purposes of the Project will be well exempted from VAT.

Overall Objective (mission):

This project did and will give further insight into the molecular mechanisms of silica structuring to enable design and synthesis of tailor made materials. Zeolite formation has been discovered to be based on self-organization of nanoscopic precursor species. Shear and convection have strong effect on this self organization process, which only can be studied under microgravity conditions.

Role of the Institute (Principal / Co-Investigator for ...):

BCo- I

V. Van Speybroeck, M. Waroquier, CMM (Center for Molecular Modeling), University Gent: Molecular Modeling of zeolite precursor aggregation on molecular level.

- Institute/University: University Gent (UG)
- Department/Laboratory: Center for Molecular Modelling
- Address: Proeftuinstraat 86, 9000 Gent, Belgium.
- Tel.: +32-9-264.65.59 Fax: +32-9-264.65.60
- Veronique.VanSpeybroeck@UGent.be

Brief description of Main Tasks:

Zeolites and ordered porous materials in general play an important technical role in sustainable industrial development. The main applications of zeolites and related material are situated in the field of catalysis, molecular separations and ion exchange. In view of the proliferation of applications, there is a continuous need for new porous materials. The goal of this project is to improve insight into the molecular mechanisms of structuring of silica with the help of organic templates to enable finally the design and synthesis of tailor made porous materials. The proposal is motivated by the discovery under conditions of microgravity, that the formation of a particular zeolite (Silicalite-1) involves self-organization processes within Ordered Liquid Phases (OLP's) of nanoscopic precursor species. Even though a full understanding of this phenomenon is not yet achieved, attempts to manipulate OLPs during synthesis already led to the development of two new classes of hierarchical materials promising high potential for applications in catalysis and molecular separation.

CHARACTERIZATION OF OLPS AND DIAGNOSTIC MEANS

Previous successful experiments under microgravity were at the origin of this proposal. The formation process of silicalite-1 investigated in sounding rocket experiments (MAXUS 4 and 5) and during the Odissea mission in 2002. An unexpected strong retarding effect of microgravity on aggregation of nanosized species into zeolite material was observed. This observation in microgravity has led to the discovery of large, precursor enriched domains playing an important role during zeolite formation. Since this indirect discovery of OLPs thanks to experimentation under microgravity, a Topical Team of several European research groups has been established. The ongoing, concerted research effort of our team led to a deeper understanding of the complex nature, ordering, and aggregation of zeolite precursor species under normal gravity conditions. The most promising state of the art diagnostic tools for our study were identified. The best way to continuously monitor development and evolution during zeolite crystallisation is a non-invasive combination of Dynamic Light Scattering (DLS) and recording of rheological properties of the fluid. To this end high frequency tools for in-situ rheology will need to be further developed and the method theoretically underpinned. These studies are best complemented with other diagnostics like Small Angle X-ray and Neutron Scattering (SAXS, SANS), NMR-, and IR-spectroscopy. Structure analysis of the finally obtained solid product allows quality assessment of the obtained materials. Theoretical modelling of inter-particle forces on different levels of interaction best complements combination of this experimental analysis. This allows the understanding of the self-organization on molecular scale as well as nano- and macroscale.

A 3D mapping of distribution of particles and concentration fluctuations on nanoscale is expected to directly link global and local observation. Currently, possible means to achieve this are explored.

MICROGRAVITY RELEVANCE AND NECESSARY DIAGNOSTICS

In previous microgravity studies it was found that microgravity appears to strongly favour the ordering and aggregation processes within the precursor suspensions. Microgravity conditions offer a unique environment where these effects can be studied in detail. The proposed microgravity experiments are essential to gain information on the rheological parameters affecting the formation of porous silicas. Ground research was necessary to understand the mechanisms of ordering and self-organisation in more detail. Over the last few years the Topical Team developed a vastly improved model for zeolite nucleation and growth. However, the role and strong influence of microgravity is still poorly understood. The accumulated expertise ensures upcoming microgravity experiments can be adequately prepared on short term. As optimum state of the art diagnostic means for in-situ microgravity studies emerged the already mentioned combination of rheological measurements combined with DLS monitoring.

While the described diagnostic strategy allows the observation of global properties like size and state of aggregation as well as onset and termination of the actual crystallisation process a spatial resolution of the ordered and precursor-enriched zones in the solution up to now is impossible. The small size of the involved species and the transient nature of concentration fluctuations which eventually result in nucleation and self-organization has up to now impeded their direct local observation. A direct 3D mapping of nanosized species in-situ is very important to link the global observations made by DLS to local processes. Development of diagnostic means to achieve this feat are currently the frontiers of research. The Topical Team has identified this development as an important medium term milestone. The final combined goal of ground based and microgravity experiments is to master the formation and behavior of specific zeolite precursors as well as their relation to the structures of the materials obtained from them.

During a scientific exchange of different microgravity users a noteworthy similarity between self-organization processes observed during protein crystallization and the above described systems emerged. From current experiments it became obvious that protein molecules first interact in the liquid phase before settling on a growing crystal. The similarity of the observations in those at first sight unrelated areas of research encouraged us to start a co-operation to probe for a general picture for the concept of self-organization during solidification from the liquid phase. The same diagnostic requirements apply for the study of self-organization of silica-nanoparticles and proteins, which makes a successful co-operation even more apparent.

TASKS

Asides an ongoing concise study of the behaviour of zeolite formation and the identification of parameters affecting the self-organization, suitable experimental environments have to be developed.

Task 1. Gaining experience in handling OLPs

A detailed experimental analysis of the impact of different parameters like, for example, temperature, dilution, chemical additives, and pH on the formed OLPs and their tendency to solidify had already been performed. In view of the planned microgravity experiments under reduced shear and flow conditions, emphasis will now be placed on the on-ground study of the effect of increased shear and flow on OLPs. Furthermore special attention will be directed to the effect of varying gravity levels during self-organization. In this context in-situ DLS measurements in a centrifuge and during a parabolic flight mission are foreseen. These studies will not only allow the definition of the most promising experimental conditions for microgravity experiments but will also support development and refinement of a theoretical model of the observed self-organization process. Main focus will be on the in-situ study of the samples with DLS and measurements of the rheological properties using high frequency techniques. Further spectroscopic means will be used to complement and verify the results. For the development of a model accounting also for shear and convection synthesis of the experimental results with theoretical insights on molecular level is necessary. The combination of experiment and Molecular Dynamic and Forcefield calculations has proven to be an excellent strategy and will be further exploited.

Task 2. Development of experimental environment

The team of scientists involved in this project is combined from experts in material sciences, rheology, DLS, sensor development and hardware development. Previous studies led to the development of an exceptionally robust non invasive viscosity sensor which now is ready to be implemented in a cell

allowing the simultaneous measurement of rheological and optical properties in a non-invasive manner. Once developed the in-situ cell now has to be calibrated and tested carefully to ensure its functionality. As a second step we developed a shear and flow cell withstanding the harsh chemical demands of the clear solutions. These in-situ cells not only are tools to characterize the studied systems with regard to the proposed microgravity experiments, they will serve as important means to translate the stated scientific requirements for these experiments into a technical solution. In the development of microgravity hardware foreseen by ESA the experience gained during the development of the in-situ cells will be indispensable. Currently the actual development of the flight hardware is expected to start in spring 2009. Only close collaboration between industry and our team will ensure the optimum experimental conditions during the microgravity and reference experiments.

Parallel to the short term preparation of the upcoming experiment the need to develop new diagnostic means to map 3D distribution of nanospecies will be addressed on medium term. A close interaction between team members familiar with the studied solutions and the experts in advanced optical diagnostics will allow pushing the frontiers of 3D imaging.

Role of the Team Center for Molecular Modeling (CMM) , Ghent University

List of the team members involved in the project:

Prof. Veronique Van Speybroeck, Prof. Michel Waroquier

2 PhD students (1 ½ financed by CMM, ½ financed by Prodex)

1 postdoc financed by IAP

Role, contribution and specific know-how, experience and suitability for the assigned activity:

Computational molecular modeling is the core activity of the applicants from Ghent University (CMM). The CMM has already a longstanding experience in modeling porous materials and the catalytic activity of these materials. Determining the active site in these catalysts and elucidating their related reaction mechanism are of paramount importance for the road to the rational design of catalysts and offering prospects of improved formulations of existing catalysts. The Leuven-Ghent team is a unique tandem for an experimental-computational approach of the template mediated formation of porous materials.

Contribution and know-how

I. Summary of the main results obtained during the period 2006-2008

One of the main contributions of the Cenoli team to the project pertains to the existence of non-standard, multi-step nucleation mechanisms mediating crystallization associated with the presence of intermediate phases. Specifically:

(i) The early stages of self-assembly in nanophase materials were explored by coupling a kinetic mean-field analysis with a lattice-based stochastic theory. A model was designed which allows the quantification of factors affecting docking efficiency of a platelet at the surface of a crystallite. Principal among these is the nature of the template itself, which is assumed to be either unstructured or bifurcated into terraces and edges/ledges. The consequences (as regards docking efficiency) of diffusive flows in the near neighborhood of a developing crystallite versus surface-only processes were assessed. Particularly in regimes where the barriers to surface diffusion are high, and/or the probability of desorption significant, it is found that three dimensional processes (leading to a "direct hit") can compete kinetically with surface-only mediated processes.

(ii) A mathematical model was proposed which accounts for reported observations on a non-standard aggregation mechanism during crystallization processes in zeolite systems, involving the mediation of intermediates consisting of a polydisperse population of nano-sized particles. The model can explain both the experimentally measured induction period in the solidification process and the final apparent equilibrium between nanoparticles and zeolite crystals. The proposed mechanism also gives insight on future experiments aiming at a more comprehensive picture of the process. The basic physical mechanisms were modelled at two levels. First, a purely phenomenological model was presented which captures the basic ideas in their simplest form. Subsequently, a more detailed and mechanistic picture was provided. This involved new concepts, such as the distribution of crystal sizes, but in the end was reduced to a system of rate equations similar to the first model. In fact, it was noted that the phenomenological model could be viewed as a systematic approximation to the more detailed model.

(iii) The construction of a theoretical scheme which could incorporate the ISS observed microgravity influence on inhibiting the self assembly of the larger intermediate nanoslabs to the zeolite crystalline state was initiated. The main idea is that the diffusion controlled mechanism in the regime of Smoluchowski-type dynamics affected by advection, anisotropic diffusivity and asymmetric nature of the intermediate nanoslabs can theoretically account for a slower binding rate of the larger intermediates. A Monte Carlo study incorporating these elements is currently under way.

II. Proposed research for the period 2009-2011

In addition to continuing the work initiated during the past 3 years, new approaches will be developed in order to incorporate explicitly in the description (a) the conditions under which the experimental studies of the Leuven team are carried out; and (b) structural factors (such as asymmetry) and geometric constraints characteristic of zeolites. An important role towards this goal will be the extensive use of molecular dynamics, Monte Carlo and kinetic Monte Carlo simulations. Specifically:

(i) *Statistical mechanical approach:* The model developed jointly by the *Cenoli* and *KULeuven* teams makes a definite prediction concerning the distribution of crystal sizes and it would seem that this could be checked via experiment. It might well be that the actual intermediates constitute a rather broad distribution of particle sizes which partly overlaps with the nanoparticle population as detected by NMR, but still differ in structure. This might explain the observed evolution of the Q4 connected silicon inside the nanoparticle population which shows a similar behaviour as of the multidisperse pre-zeolite intermediates. It is planned to focus more extensively on the connection between the intermediate phase and Qn distributions in the near future. Further extension of the model could also account explicitly for the oligomers and other mechanisms such as Ostwald ripening. Finally the role of supersaturation in the autocatalysis through formation of intermediates will be assessed.

(ii) *Crystal-size distribution:* Our recent generic model, discussed above, of nucleation and growth of crystals starting with simple (unstructured) units that eventually assemble prior to nucleation to form structured intermediates, has been developed by the *Cenoli* team in the context of zeolite crystallization in a well-stirred closed reactor. It is intended to extend this model to include spatially extended systems. Integration of the model equations will provide the crystal size distribution at different stages of maturation, which can be confronted with data from the Leuven team. Extensions accounting for spatial inhomogeneities as well as the nature of the precipitating agents and their interactions in solution will be carried out.

Milestones

Continuous activities

M1) Co-ordination of research project and integration of the results from the team members

Teams: COK

Salaries: covered by COK

Travel: 9k€ spread over 3 years asked from Prodex

M2) Experimental characterisation of molecular building units to be used in OLP studies

Teams: COK, CIT, EMAT, Tectospin, F.O.R.T.H.

COK, CIT

Salaries: 2 PhD position + 1 Postdoc positions over 3 years 100% covered by COK/CIT; 100%

Postdoc position asked from Prodex

Consumables (mostly high grade chemicals): 36k€ over 3 years, 27k€ covered by COK; 9 k€ asked from Prodex

Travel: 9k€ over 3 years; 4k€ covered by COK; 5k€ asked from Prodex

EMAT

Consumables: 51k€ over 3 years: Sample holders and liquid gases for the analysis of samples related to microgravity project

Travel: 6k€ over 3 years

M3) Co-operation with teams studying protein crystallization.

DLS measurement campaigns are already in planning.

Teams: COK, CIT

Salaries and travel: see M2;

M4) Theoretical study of molecular building units to be used in OLP studies

Teams: Cenoli, CMM

CMM

Salaries: 50% PhD

Consumables: 15 k€

Travel: 15 k€

Cenoli

Salaries: 50% Postdoc;

Consumables: 10.5 k€

Travel: 7.5 k€

M5) Development of 3D imaging of nanosized particles in suspension

Initial tests have shown 3D mapping of particle distributions and concentration gradients to be feasible. With reference samples developed in the KU Leuven the MRC aims at the development of a diagnostic facility which directly can image the self-organisation of zeolite precursors in real time.

Teams: MRC, COK, CIT

Funding will be covered in a separate project proposal with MRC as BPI.

M6) Improvement and optimization of rheology sensor

The currently available prototype viscosity sensor will be assessed for further improvement and use beyond viscosity. Among the parameters which could be optimised are surface roughness of the sensor, extension of the monitored frequency range, coupling with a low-frequency resonator and implementation of advanced signal processing

Teams: LINZ, CIT, COK

Costs: see M2

Milestones directly related to mission preparation (timeline estimation based on unofficial information by ESA)

M7) 0-6 months: Phase A feasibility study of experiment hardware

Close collaboration with industry is foreseen to ensure optimum experimental conditions

Teams: COK, CIT, LINZ

Costs: see M2

M8) 6-15 months: Phase B of hardware development

Close collaboration with industry is foreseen to ensure optimum experimental conditions;

Test samples and model samples will be prepared and fully characterised to assess performance of breadboards/prototype. Implementation of developed sensor will be followed up closely

Teams: COK, CIT, LINZ

Costs: see M2

M9) 16-24 months: Phase C of hardware development

Close collaboration with industry is foreseen to ensure optimum experimental conditions. Flight samples will be chosen and repeatedly fully characterised using flight prototype and ground based equipment.

Sensor implemented in hardware will be calibrated

Teams: COK, CIT, LINZ

Costs: see M2

M10) 2011 mission

Teams: COK, CIT

Costs: see M2

M11) Postflight data analysis

Teams: COK, CIT, F.O.R.T.H.,

Costs: see M2

Ground based study directly related to 2011 mission

M12) 0-12 months: Study of shear imposed on zeolite synthesis solutions

using the available hardware at KULeuven the effect of controlled shear during zeolite formation will be assessed. Samples will also be characterized with the whole range of experimental diagnostics.

Teams: COK, CIT, EMAT Tectospin,

Costs: see M2

M13) 3-24 months: Development and characterisation of model system of aggregation behavior of anisotropic, ellipsoidal particles

Monodisperse anisotropically shaped particles (ellipsoids and rods) have recently been synthesized and their interactions can be tuned. Their size will be optimized to mimick the situation in zeolite suspension and their behavior will be analyzed in function of convection and shear. The system will allow the development of a model for aggregation of anisotropic particles like nanosized zeolite precursors.

Teams: COK, CIT

Costs: see M2

M14) 3-9 months: Study of dense zeolite suspension using multiple scattering

An experimental setup to analyze and deconvolute light scattering from samples with multiple scattering is available. The setup will allow assessment which information can be extracted from dense zeolite suspensions. Also these samples will be exposed to shear and fully characterized.

Teams: COK, CIT, EMAT Tectospin

Costs: see M2

M15) 6-12 months: Study of increased gravity on zeolite synthesis solutions

An already available DLS setup will be installed inside a centrifuge (ESTEC) to assess the impact of increased g-levels on zeolite formation.

Teams: COK, CIT

Costs: see M2

M16) 12-18 months: Study of reduced gravity on diffusion modes in zeolite synthesis suspensions

A parabolic mission will be applied for to 1. Test hardware developed for the ISS mission and 2. To directly analyse the effect of reduced/increased gravity on the self- and collective diffusive modes in zeolite clear suspensions.

Costs: see M2

M17) 24-36 months: Synthesis of experimental and theoretical results to include convection and shear into a model of zeolite formation

Teams: COK, CIT, EMAT, CMM, Tectospin, F.O.R.T.H.

While the self-organisation of elemental units into zeolites strongly depends on convection and gravity levels, these effects cannot be explained and predicted. The microgravity results together with the molecular level forces obtained by CMM will allow the development of a model taking flow and convection into account. This model is expected to greatly benefit optimisation of zeolite synthesis in industry.

Salaries, Consumables, Travel: see M2, M4

Deliverables : Yearly reports

FINANCIAL PLAN

University Gent Ordered Liquid Phases - OLP's

Starting Date: 01.01.2009

Ending Date: 31.12.2010

Cost	2009	2010
1. Salaries: PhD grant, 50 %	20 000	20 000
2. Travel	2 500	2 500
3. Small Equipment (< 5 000 € per item)	5 000	5 000
4. Overheads (5 %)	1375	1375
Total	28 875	28 875

Table 1: Institute Costs.

TOTAL:	57 750
---------------	---------------

PRODEX EXPERIMENT ARRANGEMENT CHANGE PROCEDURE

A PRODEX Experiment Arrangement change procedure shall apply at least to any modifications of the Agency's financial commitment (Articles 2 or/and 5 of the Arrangement) and of the Term (Article 3 of the Arrangement).

1. INTRODUCTION OF A CHANGE

For all changes, whether requested by the Agency or initiated by the Institute, the latter shall submit a proposal for a PRODEX Experiment Arrangement Change Notice (ACN) on the form attached hereto. The ACN shall be filled in completely, and boxes or lines which are not applicable shall be so designated by use of the letters "NA". The form shall be signed by the Institute's authorised representative(s) and be submitted to the Agency's representative for contractual and administrative matters.

The Institute shall ensure that each change proposal is fully co-ordinated with Appendices 1 and 2 to the arrangement and that all reasonably foreseeable implications of the change have been considered. If the space on the form is not sufficient to describe the change and its consequences, the additional information shall be annexed to the form. The Institute shall, on request of the Agency, provide additional documentary evidence.

2. APPROVAL OR REJECTION OF THE ARRANGEMENT CHANGE NOTICES

Upon receipt of a ACN signed by the Institute the Agency shall consider it as regards its acceptability. Should the ACN be approved, it will be signed by the ESA Prodex Office's authorised representative and a copy be returned to the Institute. Should a ACN be rejected for any reason, the Institute shall be informed accordingly, together with the reasons for the rejection.

3. IMPLEMENTATION AND STATUS OF APPROVED ARRANGEMENT CHANGE NOTICES

Upon signature of a ACN by both parties, the ACN has immediate effect and constitutes a binding contractual agreement.

GENERAL CONDITIONS

Complementary to Article 4 of the arrangement the General Conditions applicable to all PRODEX Experiment arrangements are included in their original version hereafter (therefore, the word “contract(s)” and “contractor(s)” are to be read “arrangement(s)” and “institute(s)” respectively in the following provisions) :

PART I OF THE GENERAL CONDITIONS :

CLAUSE 1 - APPLICABLE CLAUSES AND RULES

The following general clauses and conditions shall apply to contracts placed by the Agency insofar as not stated otherwise in the relevant contract. Furthermore, specific clauses and conditions may be set out or invoked in a contract and its annexes. The annexes form an integral part of the contract.

CLAUSE 2 - APPROVAL

Offers and acceptances with regard to contracts are not binding on the Agency unless approved in writing by its Director General or his authorised representative. Unless otherwise stated in the contract the date of such approval shall be the commencing date of the contract.

CLAUSE 4 - ORIGINALS OF THE CONTRACTS

The number of originals of a contract shall be equal to the number of parties to the contract and this number shall be stated in the contract. These originals are intended for the parties to the contract.

CLAUSE 5 - AGENCY'S REPRESENTATIVES - INSPECTIONS

The Agency shall have the right to check the technical performance of the contract, and for this purpose, and for the general purpose of collaboration, the Agency shall nominate a representative(s) whose name(s) shall be notified in writing to the Contractor. Any information made available by the Contractor to such representative(s) shall be regarded as commercially confidential.

The Contractor shall, in this respect, and in accordance with any relevant security regulations, give the representative(s) of the Agency access to his premises and shall give all other necessary assistance in order that he (they) may fulfil his (their) task.

CLAUSE 7 - COMMUNICATIONS

All communications affecting the terms and conditions of the contract and concerning its execution shall be made or confirmed in writing.

CLAUSE 12 - APPLICABLE LAW

The law governing the contract shall be specified in the contract itself.

CLAUSE 13 - ARBITRATION

- 13.1 Any dispute arising out of the interpretation or execution of the contract shall, at the request of either party, be submitted to arbitration.
- 13.2 The contract shall specify the country where the Arbitration Tribunal shall sit; normally the Arbitration Tribunal shall have its seat in the country where the Contractor has his legal seat or where the contract is to be executed.
- 13.3 If no other arbitration is foreseen in the contract, any dispute arising out of the contract shall be finally settled in accordance with the Rules of Conciliation and Arbitration of the International Chamber of Commerce by one or more arbitrators designated in conformity with those rules.
- 13.4 When arbitration other than in accordance with the Rules of Conciliation and Arbitration of the International Chamber of Commerce is provided for in the contract, the procedure of the Arbitration Tribunal shall be that of the country mentioned in subclause 13.2.
- 13.5 The award shall be final and binding on the parties; no appeal shall lie against it. The enforcement of the award shall be governed by the rules of procedure in force in the state / country in which it is to be executed.

CLAUSE 14 - INFRINGEMENTS OF THE LAW

The Agency shall not be responsible if the Contractor infringes the laws or statutes of his country or of any other country whatsoever.

CLAUSE 15 - INFRINGEMENTS OF THIRD-PARTY RIGHTS

- 15.1 Unless otherwise stipulated in Part II of this document, the Contractor shall indemnify the Agency from and against all claims, proceedings, damages, costs and expenses arising from the infringement of patent rights and intellectual property rights of third-parties with respect to the subject of the contract - excluding any infringement resulting from the use of documents, patterns, drawings or goods supplied by the Agency - which may be made, or brought against the Agency, or to which the Agency may be put by reason of such infringement or alleged infringement.
- 15.2 The Agency shall notify the Contractor immediately of any written claim or notice of infringement of third-party rights which it received concerning the contract.
- The Contractor shall immediately take all necessary steps within his competence to prevent or end a dispute and shall assist the Agency to defend against, or make settlement in respect of, any claim or notice of infringement or suit for infringement. Written claims or notices of infringement of third-party rights will be accepted or met by the Agency only in agreement with the Contractor.
- 15.3 The parties shall notify each other of any known intellectual property rights connected with the use of documents, patterns, drawings and goods supplied by the one party to the other or connected with the execution of the specifications laid down by the other party.

CLAUSE 21 - FINAL SETTLEMENT

- 21.1 The Contractor shall be allowed to claim final settlement when all his obligations under the contract have been fulfilled. For the application of this clause, these obligations shall not include those of guarantee. The Contractor shall, in addition, certify whether or not any inventions as defined in Part II hereof, were made in the course of the contract.
- He shall submit a final statement in five copies.
- If the contract provides for several batches of settlement, each batch is to be paid and settled separately.
- 21.2 The Contractor shall supply the Agency with all documents specified in Annex I and necessary for payment, without explicit request by the Agency.
- 21.3 Unless otherwise provided for in the contract, a period of one month shall be granted to the Agency for the execution of the final payment. This period shall begin on a date to be stated in the contract.
- 21.4 Whenever any sum of money shall be recoverable from, or payable to, the parties, the sum may be deducted from the sum due, or thereafter becoming due, to the parties under any other contract between the parties.

CLAUSE 34 - CANCELLATION IN SPECIAL CASES

Contrary to all other General Conditions listed in this Appendix 4, Clause 34 as such is not applicable; certain situations described therein however do have the consequences laid down in Article 6 of the contract. Therefore the text of Clause 34.1 is repeated hereafter for convenience :

- 34.1 The Agency may at any time cancel the contract by giving written notice with immediate effect in any of the following events:
- a) if the Contractor becomes insolvent or if his financial position is such that within the framework of his national law, legal action leading towards bankruptcy may be taken against him by his creditors;
 - b) if the Contractor resorts to fraudulent practices in connection with the contract, especially by deceit concerning the nature, quality or quantity of the supplies, and the methods or processes of manufacture employed or by the giving or offering of gifts or remuneration for the purpose of bribery to any person in the employ of a Member State or of the Agency or acting on its behalf, irrespective of whether such bribes or remuneration are made on the initiative of the Contractor or otherwise.

PART II OF THE GENERAL CONDITIONS (CLAUSES 36, 37, 38 and 39) :

Unless otherwise agreed with all parties to arrangements concluded for the purpose of "co-operative activities" as planned in the PRODEX Programme Declarations and provided that appropriate provisions are then included in the special conditions of the arrangement in question (Article 4, Clauses 37, 38 & 39), the following general provisions 36, 37, 38 & 39 shall apply.

CLAUSE 36 GENERAL

General Rule

- 36.1 These Part II (Option A) Clauses and Conditions apply to Contracts which are also governed by the Clauses and Conditions set out in Part I. In the event of conflict between the General Clauses and Conditions in Part I and Part II (Option A) the clauses in Part II (Option A) shall prevail.
- Definitions for Part II (Option A)
- 36.2 "Agency's Own Requirements" means the activities and programmes undertaken by the Agency in the field of space research and technology and space applications in accordance with Article V 1(a) and (b) of the European Space Agency Convention;
"Agency Technology and Product Transfer Board" means the body established by the Agency Council to consider the transfer or licence of any Intellectual Property Rights or product, process, application or result arising from the Contract to an entity not Located in a Member State or to an international organisation;

"Background Intellectual Property Rights" means all Intellectual Property Rights not developed under contract with the Agency either prior to or during execution of the Contract which are used by the Contractor and/or the Agency to complete the Contract or required for use of any product, application or result of the Contract; "

Contractor" means the legal person or body who is party to the Contract; ESA/C/290, rev. 6

"Disclose" means the distribution or supply of information or Documentation to a third party without prior authorisation from the proprietor of the information/Documentation;

"Documentation" means all media on which information or data of any description is recorded including all paper documents, and electronic communications whether in electronic or hard copy form;

"Favourable Conditions" means conditions a seller is willing to sell on and a purchaser willing to accept which are more favourable to the purchaser than Market Conditions (and which normally allow reasonable profit for the seller);

"Intellectual Property Rights" means all Registered Intellectual Property Rights, and all unregistered intellectual property rights granted by law without the need for registration with an authority or office including all rights in information, data, blueprints, plans, diagrams, models, formulae and specifications together with all copyright, unregistered trade marks, design rights, data base rights, topography rights, know how and trade secrets or equivalent rights or rights of action anywhere in the world;

"Legitimate Commercial Interest" means an interest the Contractor can demonstrate which is important to its ability to commercially exploit Intellectual Property Rights arising from work performed under the Contract for a defined period of time which includes but is not limited to an economic position vis-à-vis a competitor, loss of profits or survival of an undertaking;

"Located" means belonging to a State according to the criteria set out in Article II (3) of Annex V of the European Space Agency Convention;

"Market Conditions" means conditions a seller is willing to sell on and a purchaser is willing to accept without restrictions or influence by the Agency;

"Member State" means a State which is party to the European Space Agency Convention in accordance with Article XX and XXII of the said Convention;

"Object Code" means the code for a computer programme expressed in machine readable form usually automatically compiled from Source Code by machine;

"Open Source Code" means Source Code for computer software developed under the Contract which the Contract specifies as Source Code which the Agency will distribute to members of the public free of charge;

"Operational Software" means computer programs used or required on the ground to validate and control a space mission, for calibration of data derived from a space mission or for any other Agency purpose including all updates, modifications and enhancements of such programmes which (1) are developed (or are in the process of being developed), modified, enhanced or maintained by more than one party and (2) which have an expected use for the Agency's essential purposes over a period of more than 5 years;

"Participating State" means a Member or non-Member State participating in a given Agency programme according to Article V.1 (a) and (b) of the European Space Agency Convention;

"Participating State's Own Public Requirements" means a public programme in the field of space research and technology and their space applications fully funded or funded to a substantial extent by the Participating State;

"Persons and Bodies" means any individual, partnership, company, research organisation or legal entity under the jurisdiction of a Participating State which, when relevant, meets the criteria set out in Article II (3) of Annex V to the European Space Agency Convention;

"Registered Intellectual Property Rights" means all rights granted by law through registration with an authority or office (whether actually registered or in the form of applications) including all registered patents, utility models, designs, topography rights, domain names and trade marks or equivalent rights and rights of action anywhere in the world;

"Source Code" means the code for a computer programme expressed in human intelligible form which can be compiled automatically into Object Code by machine;

"Source Code Agent" means the Agency or an independent body which the parties agree can hold software Source Code secure for release upon the events specified in clause 42;

"Subcontractor" means a third party who enters into a written agreement with the Contractor for a defined research and development task required for completion of the Contract.

Interpretation

- 36.3 If an issue arises over the interpretation of Favourable Conditions, Market Conditions and/or Legitimate Commercial Interest any party requiring access and use of Intellectual Property Rights arising from work performed under the Contract may request a reasoned binding opinion from a forum agreed by the parties (and if the parties cannot agree on a forum the matter shall be referred to the Agency).

Contractor Employees/Service Providers

- 36.4 The Contractor shall ensure that all work to be performed under the Contract is carried out by persons who have a written agreement with the Contractor and that when lawful the agreement includes provisions that ensure:

- (a) all Intellectual Property Rights in results, information, data or Documentation arising from work performed during the course of their engagement shall be owned by the Contractor; and
- (b) all results information, data and Documentation obtained for the purpose of the Contract will only be circulated under terms which comply with the Contract.

Subcontract Clauses

- 36.5 If the Contractor requires the services of a Subcontractor for the purposes of fulfilling obligations under the Contract the Contractor may enter into subcontracts with the approval of the Agency unless otherwise specified in the Contract. Each subcontract shall provide:

- (a) the Subcontractor with the same rights and obligations in relation to work performed under the subcontract that the Contractor has agreed to in relation to work performed under this Contract and in particular shall ensure that only the Subcontractor has the rights and obligations set out under clause 36.3 (Interpretation), clause 36.4 (Contractor Employees/Service Providers), clause 39 (Ownership of Intellectual Property Rights), clause 40 (Registration of Intellectual Property Rights), clause 41 (Use of Intellectual Property Rights), clause 42 (Software), clause 43 (Background Intellectual Property Rights), clause 44 (Exploitation), clause 46 (Fees) and clause 49 (Transfer outside Member States);
- (b) for the exceptional case when work is carried out jointly by the Contractor and one or more Subcontractors, the parties will agree to normally vest the ownership of the intellectual property rights in the principal contributor to the development, provided the principal

contributor is able and willing to exploit such rights and compensation in form of a licence and/or payment is agreed. In such case, the assignment shall be notified to the Agency and the subcontract shall be drafted to comply with these provisions of this Part II (Option A).

- 36.6 To assist in the identification of Intellectual Property Rights created and owned by the Subcontractor each subcontract shall define in writing the product, application or results arising from work performed under the subcontract.

CLAUSE 37 INFORMATION TO BE PROVIDED

Contract Reports

- 37.1 The Contractor shall provide regular reports detailing all work performed under the Contract as specified in the Contract. The reports shall provide details of all work undertaken and completed, any current or anticipated problems in completing the Contract, the progress achieved and whether any results or Intellectual Property Rights arising from work performed under the Contract have been (or are expected to be) exploited.
- 37.2 The Contractor shall draft a final report detailing all results of the Contract as specified in the Contract. The Agency may make the report available to Participating States and Persons and Bodies. For the purpose of the report the Contractor shall provide the Agency with relevant commercially sensitive information, data, results and Documentation which shall be included in a separate part of the report marked "Proprietary Information" only to be circulated with prior written consent from the Contractor (such consent not to be unreasonably withheld taking into account the Contractor's Legitimate Commercial Interest).
- 37.3 If requested by the Agency, and at the Agency's reasonable expense, the Contractor shall provide the Agency with any additional information, results, data or Documentation arising from work performed under the Contract not included in reports provided to the Agency together with any related information the Agency may reasonably require for the Agency to use or make available in accordance with the Contract.

Access to Information

- 37.4 Information, data and results arising from work performed under the Contract shall be reported to the Agency who may make such information, data and results available for Participating States and Persons and Bodies to use on the condition that Participating States and Persons and Bodies comply with the terms on Use of Intellectual Property Rights (set out in clause 41) and on Disclosure (set out in clause 38).

CLAUSE 38 DISCLOSURE

- 38.1 The Contractor shall not Disclose any Documentation obtained from the Agency which is marked as "Proprietary Information". The Contractor shall only circulate such Documentation to its employees that require that Documentation for the purposes of complying with the Contract. The Contractor shall never circulate such Documentation to those not employed by the Contractor (other than in compliance with these Clause and Conditions) without prior written consent from the Agency in which case the Agency may require the recipient to sign a non-disclosure agreement.
- 38.2 The Agency shall not Disclose any Documentation obtained from the Contractor which is marked "Proprietary Information". The Agency shall only circulate such Documentation to its employees that require that Documentation for the purpose of complying with the Contract or for using, modifying or maintaining any product, application or result of the Contract and the Agency shall never circulate such Documentation to those not employed by the Agency (other than in compliance with these Clauses and Conditions) without prior written consent from the Contractor in which case the Contractor may require the recipient to sign a non-disclosure agreement.
- 38.3 The obligations in clauses 38.1 and 38.2 shall not apply to Documentation:
- which at the time of circulation has already entered the public domain or which after circulation enters the public domain other than through a breach of this Contract;
 - which at the time of circulation is already known by the receiving party (as evidenced in writing) and is not hindered by any obligation not to circulate;
 - which is later acquired by the receiving party from another source and is not hindered by any obligation not to circulate;
 - which is required to be circulated by law or order of a court of competent jurisdiction.

CLAUSE 39 OWNERSHIP OF INTELLECTUAL PROPERTY RIGHTS

- 39.1 The Contractor shall own all Intellectual Property Rights and have the right to apply for and to own any Registered Intellectual Property Rights arising from work performed under the Contract. At the Contractor's request and expense the Agency shall carry out all reasonable tasks including executing any document required to vest such title in the Contractor.
- 39.2 The Agency shall be granted the rights, including the access, to Intellectual Property Rights set out in clauses 39 to 44 and reserves the right to require the Contractor to assign Intellectual Property Rights arising from work performed under the Contract in the case of:
- the Contractor's failure to apply for registration or the Contractor's abandonment of Registered Intellectual Property Rights arising from work performed under the Contract (as set out in clause 40.4 and 40.5);
 - the Contractor's failure to exploit (as set out in clause 44.2);
 - Operational Software (as set out in clause 42.7);
 - Open Source Code (as set out in clause 42.9).
- 39.3 When the Contractor assigns any Intellectual Property Rights arising from work performed under the Contract he shall give notification to the Agency within 4 weeks of the date of assignment.
- 39.4 The Contractor shall ensure that any assignee of Intellectual Property Rights arising from work performed under the Contract complies with the same obligations (including the obligation to exploit the Intellectual Property Rights) and grants the Agency, Participating States, Persons and Bodies the same rights that the Contractor has agreed to under this Contract.

ANNEX I TO THE GENERAL CONDITIONS

CLAUSE 9 - LIMITATION OF LIABILITY

- 9.1 The limit of liability is an amount to be stated in the contract, which shall be the maximum amount to which the Agency is committed and which can only be increased by a written agreement of the Agency.
- 9.2 If at any time the Contractor has reason to believe that the commitments which he will incur in the performance of the contract in the next succeeding sixty (60) days, when added to all costs previously incurred, will exceed seventy-five percent (75%) of the limit of liability, the Contractor shall notify the Agency in writing to that effect, giving the revised estimate of the total cost.
- 9.3 The Agency shall not be obliged to reimburse the Contractor for costs incurred in excess of the limit of liability and the Contractor shall not be obliged to continue performance under the contract or to incur costs in excess of the limit of liability, unless and until the Agency shall have notified the Contractor in writing that such limit has been increased up to a revised amount. Any costs incurred by the Contractor in excess of such limit prior to the approval of the increase shall be allowable to the same extent as if such costs had been incurred after the increase.

CLAUSE 10 - RIGHT TO AUDIT

The Agency reserves the right to audit, either itself or through an authorised representative, the claim of the Contractor, for cost incurred in the execution of any cost-reimbursement type contract or any contract with ceiling price to be converted into a fixed price which according to the provisions of Clause 3.4 is to be treated as a cost reimbursement contract.