

External Review of the DST/NRF CoE in Catalysis, University of Cape Town – March 2009

The purpose of this document is to provide the NRF with information on the achievements of the DST/NRF Centre of Excellence, *c*change*, at the University of Cape Town, and to make recommendations for the future.

Executive Summary

*c*change* is a lively, extremely well managed network that has succeeded in bringing all academic groups in heterogeneous, homogeneous and biocatalysis as well as catalytic reaction engineering together on a subject of key importance to the South African society. Almost all the targets set at its inception have been realized. *c*change* is at present a network of expertise. The Review Panel fully supports this approach at this stage and strongly recommends that *c*change* will be enabled to continue its activities in the future while striving to achieve international excellence in selected programs. We are very impressed by the enthusiasm and morale of staff and students at all levels within *c*change*. The concept of Centres of Excellence and the manner in which it is driven by the DST and NRF deserve governmental support and acclamation.

Background

The review panel consisted of

- Prof Dragomir B. Bukur, Joe M. Nesbitt Professor of Chemical Engineering, Texas A&M University at Qatar
- Prof J.W. (Hans) Niemantsverdriet, Schuit Institute of Catalysis, Eindhoven University of Technology, Eindhoven, The Netherlands
- Prof Helgard Raubenheimer, Department of Chemistry and Polymer Science, University of Stellenbosch, (Convener)

The review took place on 23-25 March 2009 at the Department of Chemical Engineering, University of Cape Town, where the panel and Ms Anke Rädcl of the NRF, were received by the Director of *c*change*, Prof M Claeys, and its Administrator, Dr R Weber. We were joined by Dr A Kanicke, Executive Director of Knowledge Fields Development at the NRF, who explained the process and the terms of reference. From here onwards, the program proposed by the Centre (Addendum 1), was essentially followed.

All dealings with the NRF were handled in a professional manner and all documents received were complete.

At UCT, the panel members were treated with great courtesy and frankness at all times and no restrictions were placed on their enquires. The three members of the panel worked extremely well together and this report represents their combined opinions.

The panel also found the Self Evaluation Report by **c*change** a complete, fair and honest portrayal of the present situation.

In the rest of this report the seven Key Performance Areas in the Terms of Reference are addressed separately followed by Further Comments and Recommendations.

Report

1. Research

Being the main activity of a CoE, this performance area is treated in relatively great detail.

The research activity consists of four major Programmes, selected to enable the integration of the various directions in catalysis (hetero-, homo-, bio-, engineering-) as well as the existing expertise in the country, while being at the heart of the needs of South Africa's chemical process industry.

1.1 *The Syngas Programme*

Participating institutions	UCT, WITS, UL*
Academics involved (ca)	9
Postdocs	1
PhDs	3
MScs	10
Publications 2005-2008 [IF > 1] (Cross disciplinary)	5(2)
PhDs (and MScs) graduated in 2006 and 2007	3(1)

This programme focuses on the conversion of synthesis gas (CO + H₂) into methanol, olefinic, paraffinic and oxygenated hydrocarbons, with the objective to understand and influence product selectivity. The **c*change** members collaborate with several institutes outside the network.

This is an excellent, well thought out programme, with sufficient critical mass to be internationally competitive. Interdisciplinary successes have been achieved. The truly unique and highly sophisticated laboratory reactor infrastructure at UCT

* At UCT (Chemistry and Chemical Engineering), Stellenbosch (Chemistry and Chemical Engineering) and University of the Free State (Chemistry and Microbiology) two departments each are involved; for the rest only one (Chemistry).

rates amongst the best in the world. Frequent contacts with SASOL and PetroSA, together with substantial expertise within the centre makes this programme eminently suited to become an international centre of excellence in this area. Intensive collaboration with the best scientists in the world in this area would be beneficial and should be established. Catalyst preparation from a materials science viewpoint deserves more attention in future.

1.2 *The Paraffin Activation Programme*

Participating institutions	UCT, US, UKZN, UFS
Academics involved (ca)	7
Postdocs	3
PhDs	3
MScs	8
Publications 2005-2008 [IF > 1] (Cross disciplinary)	(7)2
PhDs (and MScs) graduated in 2006 and 2007	(3)

The activities in this programme deal with the activation of the relatively unreactive alkane backbone of saturated hydrocarbons by introducing hydroxyl, carboxyl, carbonyl or olefinic functions at the terminal carbon of the chain. This is a genuinely challenging and high risk programme, with the potential for very high rewards if the project is successful. The objectives are clear and well defined. The approach is to use heterogeneous, homogeneous and biocatalysis in a biomimetic strategy where enzymes provide inspiration for the design of new catalysts. The advantage of the programme is that it rests on a truly multidisciplinary approach. **c*change** allowed the establishment of a viable research group at UFS that would have been impossible to finance through the normal channels. Completely new coordination chemistry research has been initiated at UKZN because it was deemed necessary for one of the subprojects within this programme. We note that there is very limited heterogeneous catalysis activity in the program. Thus far, progress has been slow, which is understandable and acceptable for such a new and challenging venture. The panel strongly recommends that national (e.g. Prof H Marques, SA Research Chair at Wits) and international contacts be established to assist in guiding this challenging programme.

1.3 *The RSA Olefins Programme*

Participating institutions	UCT, US, UJ, NWU, UFS
Academics involved (ca)	8
Postdocs	2
PhDs	-
MScs	13
Publications 2005-2008 [IF > 1] (Cross disciplinary)	20(2)
PhDs (and MScs) graduated in 2006 and 2007	1(1)

The Olefins Programme aims at adding value to the typical odd-numbered alkene feedstocks which are formed in the Fischer-Tropsch process. The programme is

well defined and rests heavily on homogeneous catalysis and therefore serves as a highly suitable training ground for students in homogeneous catalysis. It is also the most productive programme as far as publications and numbers of MSc graduates are concerned. However, internationally there are many activities in this area and establishing prominence and scientific leadership will be difficult. Apart from a few exceptions, the overall approach and methodology have been of fairly routine nature. Very little interdisciplinary interaction has been achieved. The national value of the programme, and the aspect of student training nevertheless make this programme worthwhile.

In order to achieve satisfactory goals for a centre of excellence, it is recommended that more innovative and higher risk approaches be introduced. Heterogeneous catalysts should also be considered in attempts to cross the existing borderlines between disciplines.

1.4 *The Small Volume Chemicals Programme*

Participating institutions	UCT, NMMU, US, UFS
Academics involved (ca)	6
Postdocs	1
PhDs	1
MScs	4
Publications 2005-2008 [IF > 1] (Cross disciplinary)	3
PhDs (and MScs) graduated in 2006 and 2007	1(1)

We are less impressed with the fundamental content and originality of this programme relative to the others. This programme originally aimed at the functionalization of phenolic waste streams from coal gasification, and has relied largely on known chemistry. However, we were pleased to learn that the programme is likely to be redefined into the direction of microreactor technology, with the aim to enable small scale specialty chemicals production. We strongly support this idea as well as the plans to seek collaboration with the international leaders in this area (e.g. Holger Loewe, Volker Hessel, at IMM Mainz). Microreactor technology is a field where IP generation and entrepreneurial activities are conceivable.

General remarks

For all programmes it is too early to judge their success. The overall number of publications in most programmes is still modest as can be expected for the short time that **c*change** has existed. Nonetheless, there has been a significant increase in the number of publications during 2008, particularly in the Olefin Programme. A pertinent goal should also be to increase the number of publications in higher impact journals.

It is pleasing to see that the demographic HR targets have been realized, although we noticed the occasional concern that highly qualified talented candidates could not be accommodated due to strict demographic targets.

Despite the programmes being gender neutral, the numbers and quality of female academics and students are impressive.

2. **Education and training: HR development**

c*change appears to function remarkably well as a platform where students meet and collaborate. All students we met (about 10 from different universities) echoed this message with great enthusiasm. The annual **c*change** symposium where all students report on the progress of their work is seen as a great success and an excellent opportunity to broaden one's horizon by being exposed to other disciplines that are relevant to catalysis. Several students spent time at partner locations to use equipment there. One student described **c*change** as a nice collaborative umbrella which stimulates people to make contact across disciplines.

Students told us that they had been able to attend international conferences abroad with financial support from **c*change**.

Although, the employment of postdocs is an expensive venture, the important role of such a programme should not be underestimated and we strongly support attracting them into the research programmes. They not only provide the necessary support to young researchers or within large groups but also the opportunity for effective knowledge and expertise transfer from respected groups overseas.

Targets for racial and gender disparity have been realized. Although we understand that such targets are a fact of life in South Africa, we also have some concern that rigid targets may slow down the progress towards achieving excellence if sufficiently competitive students from one or other designated group cannot be enrolled.

We conclude that the **c*change** CoE is still growing and can now afford to be even more selective in terms of student acceptance. While meeting demographic and gender targets, the duration times agreed upon could also be adhered to.

We do have some concerns:

- Sufficient funds are not available to increase and maintain the development of young researchers
- Too large numbers of students are placing constraints on budgets
- Some excellent students were not accepted due to demographic constraints

3. **Knowledge brokerage**

Good progress has been made with certain initiatives of *internal* knowledge sharing. The **c*change c*symposium** held annually since 2005 have been a great

success with academics and students alike. We have already commented upon successful student exchange as a means of knowledge transfer. Plans are in place to set up a virtual modular catalysis course at MSc level and to broaden the access to molecular modeling facilities amongst partner institutions. Fruitful contacts may be established with the Netherlands Organization of Catalysis Research (NIOK) and the Leverhulme Centre for Innovative Catalysis in Liverpool as both organizations have run integrated courses on catalysis for more than 15 years. Such a newly-developed course could be valuable for students outside South Africa as well.

We were also impressed with the service rendered *outside of c*change*. These involvements include the organization of Schools' Days and the development of material for a Chemical Processing module designed for high school teachers and learners, exemplifying valuable contributions to society.

4. **Networking**

The internal networking is very active with the already mentioned annual **c*change** symposium, connected to the CATSA conference, as a highlight. The CATSA conference itself has benefitted networking as well and now presents a broad spectrum of activities in catalysis, with contributions from homogeneous, heterogeneous and biocatalysis, and has grown to 250 delegates, 30 of which come from abroad. This is certainly a measure of success!

Also in the research areas, examples presented to us confirm that students and supervisors visit partner locations and hold teleconferences. There is no doubt that **c*change** with a center of gravity at UCT, is an effective national network.

International contacts exist with St Andrews, Gent, Oldenburg and a number of German Scientists but have to be developed according to the existing plans.

We specifically recommend that attempts be made to: (a) involve certain of the scientists that were recently awarded SA Research Chairs; (b) explore establishment of collaboration with the following individuals or groups:

- Heterogeneous catalysis (fundamental): Denmark (DTU) and Berlin (Fritz-Haber-Institute)
- Heterogeneous catalysis (applied): Prof A. Corma (Valencia, Spain)
- Molecular modeling: use the Eindhoven connection of Sasol, or explore contacts with the Norskov Group at DTU
- Homogeneous catalysis: expand contacts with St Andrews (Cole-Hamilton); consider inclusion of Leibniz Institute, Rostock/Berlin (M. Beller), Max Plank Institute (Mülheim), W Leitner (Aachen), S. Mecking (Konstanz).

5. **Service rendering**

Similar to the situation in Departments at Universities, it is expected that particular services in the Education and Business Sectors are rendered by members who are recognized experts in certain fields. We judge that such functions are certainly performed at an adequate level by various scientists within **c*change**. The expertise gained in running the Centre, provides valuable experience for certain members to then act in advisory capacity during the establishment of other centres and research units.

6. **Management**

The governance and management structures put into place by **c*change** structures are efficient and boost strife-free collaboration. The reporting structures in terms of finance, capacity building and compliance to rules – particularly pertaining to the accommodation of students from the designated groups – are simple but unambiguous and generate quick responses from physically removed centres of activity. Although most of the academic members also engage in research outside **c*change**, those activities are clearly excluded in the reporting documents making performance evaluation relatively easy.

Michael Claeys and Rein Weber have to be commended for the manner in which they lead **c*change** and Jack Fletcher for setting it up. The centre of gravity at UCT is well placed and logical in terms of strength, experience and commitment of the University (as expressed and illustrated to us by the Deputy Vice Chancellor (Research) – and Board Chairperson – Prof D Visser).

The four Programme Managers as well as the KPA Managers are all enthusiastic and deeply involved and committed to the goals of the programmes and Centre. Despite a low and successful leveraging of 20% administrative cost, the funding has probably not kept pace with the growth of the Centre or inflationary pressures.

We are satisfied that planning for the future – and especially measures to manage the presence of two centres in one location – is taking place.

7. **DST/NRF CoE Programme**

All members of the panel agree that the concepts of physical or virtual centers, based on existing strength, in areas of strategic importance for South Africa makes a lot of sense. However, the programmes in these centres should primarily be seen as efforts to concentrate resources and make these available nationally, as well as to educate larger numbers of students in areas that are strategically important for the country on an internationally competitive level. In our opinion, this does not necessarily imply that the research should be at the international forefront right from the beginning. Qualifications such as ‘excellence’ should at first be considered in a national or regional context. It takes many years and in

general high levels of funding to bring a new research program at the internationally competitive level. It would be unfair to request a new center to be at the forefront in a period less than the time it takes to educate three generations of PhD students: the first to build up new capacity and competences, the second to explore these, and the third to harvest. Postdoctoral students with relevant experience may accelerate such developments, but hiring them has significant budgetary consequences.

The funding given to ventures such as **c*change** is very modest, and not at all in line with expectations that a true Centre of Excellence will eventually evolve. Particularly more capital funding for unique equipment would be needed. It is by all means understandable that budgetary limitations in general diminish the desirable funding to the level of seed money, providing opportunity to the members to leverage funding from their own institutions – and this possibility has already played an important role in the establishment of infrastructure. But since, as mentioned, more capital funding for unique equipment is needed, the Funding Agency should feel a strong responsibility to assist in finding and opening additional sources of financial support in selected cases of severe need. Without such possibilities, expectations that the newly founded centre will rise to the level of excellence in all of its programs are unjustified and can only lead to the disappointment of the Funding Agency and the frustration of hardworking and committed scientists who are asked to achieve the impossible.

General Conclusions and Recommendations

C*change is a professionally led virtual centre with admirably well-functioning management procedures and structures in place for meeting, reporting and planning in which the whole network is finally involved. It is rare to experience such a professional and well-functioning organization in academic networks.

The effective reporting structure immediately reveals that **c*change** has in general been quite successful in achieving its key performance targets as agreed upon in the Service Level Agreements and that the research programmes can in general be qualified as highly relevant for South Africa. They are clearly inspired by strengths in the South African chemical process industry, and in certain areas – notably syngas – the research occurs at an internationally recognized level.

Commendable activities in service rendering and information brokerage as a societal responsibility are taking place, although some of these activities (refereeing, participating in advisory boards etc) should be seen as standard responsibilities of academics. Particularly noteworthy is the development of a science teaching package aimed at providing teachers of secondary schools with teaching materials and practical projects.

In all fairness, one cannot claim that **c*change** is a centre of excellence on the international scene. Publication output, impact and interaction with international stars in the field are all on a modest level. However, it takes time to achieve goals of excellence, and expecting this to have happened in the four years since inception is unrealistic. Our

recommendations relating to further and more intensive national and international collaboration, should be taken seriously. Such involvement is also important for benchmarking and planning.

Naturally, there are concerns with respect to the future as well. Firstly, the retirement of one very active UCT member and the upcoming retirement of two internationally visible professors at the University of Witwatersrand, will be a severe loss for **c*change**, particularly because clear plans for succession are probably not in place. Secondly, the establishment of a large centre on hydrogen technology, with UCT as home base, may occur at the expense of **c*change** if both centers will be competing for the same students and the commitment of the academics. While members of the Board have mixed feelings about the H2 Competence Centre and the effect it will have on the present staff, both Directors are confident that the process can be managed and synergy achieved within the CatCentre. We recommend continuous discussions with (and involvement of) the Board and stakeholders of **c*change**.

We strongly support **c*change**'s initiative to obtain additional grant funding, particularly for expensive equipment plus a once-off start fund towards the development of young researchers from designated groups within the center. Simultaneously, downsizing the number of students with the concomitant availability of more money for running costs should be implemented as proposed.

As mentioned in the SWOT analysis (Self Evaluation Report) the production of more joint publications should become a serious goal to achieve.

Our final recommendation to the DST and NRF is to cherish the impressive achievements of **c*change** and to continue and possibly expand its funding. This centre is offering excellent value for money in an area that is of the utmost importance to the South African economy – present and future.

Review of the DST-NRF Centre of Excellence in Catalysis

PROGRAMME

Period: 23 – 25 March 2009

Venue: Centre for Catalysis Research
Department of Chemical Engineering (Level 5)
South Lane, Upper Campus
University of Cape Town (UCT)
Rondebosch, Cape Town

Day 1 (Monday 23 March) Venue: **Tanzanite Room** (Level 5)

09h00 – 10h00: Briefing by NRF representative

10h00 – 11h00: Review panel closed discussion

11h00 – 11h15: Coffee / Tea Break

11h15 – 13h00: Interview with Director (A/Prof. Michael Claeys) and Administrator (Dr. Rein Weber)

13h00 – 14h00: Lunch & panel discussion time

14h00 – 15h45: Interview with Management Team
(A/Prof. Michael Claeys [UCT/Dir & SYN], Prof. Sue Harrison [UCT/PAR],
Prof. Ben Zeelie [Nelson Mandela Metropolitan University/SVC & SR],
Prof. Manie Vosloo [North West University/WU/OLE], Mr Stephen Roberts
[UCT/KB], Dr Rein Weber [UCT/Admin])

15h45 – 16h00: Coffee / Tea Break

16h00 – 16h15: Interview with Schools Curriculum Development Officer (Mrs Rene Toerien)

16h15 – 17h00: Review panel closed discussion

Day 2 (Tuesday 24 March) Venue: **Board Room** (Level 5)

09h00 – 09h30: Review panel closed discussion

09h30 – 11h00: Interview with postgraduate students and postdoctoral fellows - A. Hughes [UCT PhD/PAR], N. van der Bergh [UCT PhD/PAR] N. Fischer [UCT PhD/SYN], R. Brosius [UCT P-Doc/SYN], N. Mungwe [ex-University of the Western Cape MSc/OLE], R. Malgas [University of the Western Cape & Stellenbosch University PhD/OLE], N. Antonels [UCT-Chemistry

ADDENDUM 1



MSc/OLE] C. van der Merwe [UCT MSc/SVC], Nicola Toma [UCT PhD/SYN], P. Mogorosi [UCT PhD/SYN]

- 11h00 – 11h15: Coffee / Tea Break
- 11h15 – 13h00: Interview with project leaders (M. Smit [University of the Free State/PAR & SVC], H. Friedrich [University of KwaZulu-Natal/PAR], S. Mapolie [University of Stellenbosch/OLE], J. Moss [UCT/PAR & OLE & SYN], E. van Steen [UCT]/SYN, L. Callanan [University of Stellenbosch/SVC], M. Scurrall / N. Coville [University of the Witwatersrand/SYN – telephone conference if required])
- 13h00 – 14h00: Lunch & discussion with DVC Research & Board Chairperson [Prof. D. Visser]
- 14h00 – 15h30: Interview with c*change Board Members [Prof J. Fletcher (ex-Director), Mr P. Gibson (Sasol), Dr. M. Mdleleni (PetroSA) and Dr T. Bromfield (Sasol & Rep. for participating institutions)]
- 15h30 – 15h45: Tea / Coffee Break
- 15h45 – 16h15: Tour of the facilities
- 16h15 – 17h00: Follow-up discussion with Director (A/Prof. Michael Claeys) and Administrator (Dr. Rein Weber)

Day 3 (Wednesday 25 March) Venue: **Tanzanite Room** (Level 5)

- 09h00 – 10h00: Review panel closed discussion / Report writing
- 10h00 – 10h30: Optional follow-up discussion with Director (A/Prof. Michael Claeys) and Administrator (Dr. Rein Weber)
- 10h30 – 11h00: Tea / Coffee Break
- 11h00 – 13h00: Report writing
- 13h00 – 14h00: Lunch
- 14h00 – 17h00: Finalisation of Draft Review Report

PAR – Paraffin Activation Programme
OLE – RSA Olefin Programme
SYN – Synthesis Gas Programme
SVC – Small Volume Chemicals Programme
KB – Knowledge Brokerage
SR – Service Rendering