CURRICULUM VITAE --- Dr Jan Andries Pretorius (ID: 491116 5001 086)
PhD: Synergism in Metal Extraction (1978), UNISA

Research background

Thirty year experience in the Petro-Chemical Industries of South Africa and the United Kingdom focussed on the development of novel chemical routes and scaled process design for the mining industry, commodity and petro-chemicals, including aroma chemicals.
These investigations also supported by software development of:

a) Laboratory instrumental control (automation) – specific applications
b) Online process control, statistical and physical chemistry algorithm development
c) Simulation in X-Ray diffraction including
d) Finite Element behaviour and predictions of commodity components in the mining explosives regime

Achieved **six** chemical process plant and **two** mining explosive process automations.
Full member of the ICI (UK) Laboratory Automation and Simulations Panel (1984 – current).
Member of the International Catalyst Modelling Consortium, hosted from San Diego, USA by Biosym Inc. (1991 – 2000) --- now Accelrys.

Joined the PBMR Research team at University of Pretoria (Chemistry Department) in August 2006, to investigate optimum material composites and design of the PBMR-reactor -- the project was officially closed in 2009. Following the PBMR project closure, converted the main PBMR-Cluster computer to an academic facility and established a material science interest group, culminating in formal material science research modelling ventures in the Departments of: Chemistry, Physics, Chemical Engineering and Material Sciences at University of Pretoria. University of Pretoria now also a formal member of the International *Materials Design* Modelling Consortium (workshop) hosted from Paris, France.

Research Interests (current)

a) Development of specialized single-atom Quantum Chemistry software to simulate ionization potentials, electron affinity and optimum atomic potentials, derived from the original *Atomic Condensed Radii* concept derived by prof Jan Boeyens.
b) Soon to commence on a more intense Quantum Chemical software design, based on the principle of Matter Waves (wave mechanics).
c) In the process of converting a previously developed Thermodynamics species-based analysis software system, as UP-Central Cluster-based package, based on the theory of *Elemental Potentials*.

Application modelling (current)

1) Optimizing glassy conglomerates to capture nuclear waste (vitrification) – NECSA (PhD student)
2) Postulate high temperature binary metal alloys of Ti-Pt systems (Material Sciences Dept., UP, MSc student)
3) Graphite, water dispersed systems as advanced lubrication media (Mech. Eng., UP, MSc student)
4) Explore Bentonite clays as adsorbent for selective lubricants or carrier for pesticides (control of malaria, PhD student)
5) Water adsorbed metal surfaces and their selective susceptibility for sealants (own research)

Publications

18 Peer reviewed publications (Metal Organic, Structural, Extraction, Automation of X-Ray and related instrumentation & Chemical Modeling)
6 Conference papers (international)
3 Review papers (national/international)
16 AECI Publications + number of International ICI UK reviews, submitted through the ICI Laboratory Computing Panel (UK).
6 Internal CSIR Publications (Computational Modeling and process Chemistry --- 1999 onwards).
1 International Court paper – iso-Cyanuric Acid (1997)

INTERNATIONAL papers/presentations

1 Crystal Structure of cis-bis[1-(2-thienyl)-4,4,4-trifluoro-1,3 butanedionato]-bis(4-methylpyridine)nickel (II).
J.A.Pretorius & J.C.A.Boeyens, *J. Cryst. Mol. Struct. (1976)* ***6****, 169-176.*

2 X-ray and Neutron Diffraction Studies of the Hydroquinone Clathrate of Hydrogen Chloride.
Jan C.A.Boeyens & Jan A. Pretorius, *Acta Cryst., (1977),****B33****, 2120-2124*.

3 X-Ray Structure of two Analogues of the Carbohydrate Moeity of the Polyoxins
J.C.A.Boeyens, A.J.Brink. R.H.Hall, A.Jordaan and J.A.Pretorius, *Acta Cryst. (1977)* ***B33****, 3059-3066*

4 Structural Aspects of Synergistic Extraction – I
Crystal Structure of Bis[1-(2-thienyl)-4,4,4-trifluoro-1,3-butanedionato]Copper(II),
Jan. A. Pretorius & Jan .C.A.Boeyens, *S. Afr. J. Chem. Vol.* ***30****, (1977), 153*

5 Structural Aspects of Synergistic Extraction – II
The Crystal Structure of Cis-Bis[1-(2-thienylL)-4,4,4-trofluoro-1,3-butanedionato]-Bis(4-methylpyridine) Co(II), Cu(II) and Zn(II).
Jan. A. Pretorius & Jan. C.A. Boeyens, *J. Inorg. Nucl. Chem. (1978),* ***40,*** *407-416*

6 Structural Aspects of Synergistic Extraction – III
The Crystal Structure of *Cis*-Bis[1-(2-thienyl)-4,4,4-trifluoro-1,3-butanedionato]- Bis(methanol) Co(II) and Zn(II).Jan. A. Pretorius & Jan. C.A. Boeyens, *J. Inorg. Nucl. Chem. (1978),* ***40****, 1519*

7 Structural Aspects of Synergistic Extraction -- IV
Crystal structures of the pyridine adducts of the Co(II), Ni(II), Cu(II) and Zn(II) complexes of thenyoltrifluoroacetone and of trifluoroacetate and their extraction properties.
Jan. A.Pretorius & Jan. C.A.Boeyens. *J. Inorg. & Nucl. Chem. (1978),* ***40****, 1745*

8 Trans- en Cis-invloed in metaalkomplekse van die eerste oorgangsreeks
J.A.Pretorius – *S. Afr. Tydskr. vir Nat. Wet*. (1978), Jaargang **18**, Nr.2, 121-136.
(**Trans- and Cis-Influence in Metalcomplexes of the First Transition Series**, (Article in Afrikaans).
S Afr. J. of Nat. Science and Techn. (1978) Vol. ***18****, No. 2,121-136)*

9 Crystal Structure of Euryopsonol
G.R.Woolard, J.A.Pretorius, P.C.Coleman & D.E.Rivett. J.C.S.Perkin II (1979), **7**, 930.

10 Synthesis and Crystal Structure of 1,4,6-tri-O-acetyl-3-O-1'(R)-C-carboxyethyl-D-glucose 2', 2-lactone.
J.H.Jordaan, J.J.Nieuwenhuis and J.A.Pretorius. *S. Afr. J. Chem. (1979),* ***32****, 173-176.*

11 Crystal Structure of Retrorsine
P.C.Coleman, E.D.Coucourakis and J.A.Pretorius, *S. Afr. J. Chem. (1980),* ***33****, 116-119.*

12 Crystal and molecular structure of a pentameric carbohydrate dibutylstannylene: methyl 4,6-O-bezylidene-2,3-O-dibutylstannylene-a-D-mannopyranoside, C.W. Holzapfel, J.M.Koekemoer, F.C.Marais, G.J.Kruger and J.A.Pretorius. *S. Afr. J. Chem. (1982),* ***35****(3), 80.*
---> (The largest organic molecular structures [a pentamer sugar] ever solved by *Direct Methods*)

13 Upgrade of the Control Hardware and Computer Software of an X-Ray Powder Diffractometer.
J.A.Pretorius (Paper presented in Hamburg at the XIIth International Crystallographic Conference).
Acta Crystallographica Section A, 40: C411-C411 Suppl. S 1984

14 **Formation of a homoleptic unbridged metal-metal bonded isocyanide dimer of Ruthenium(I) by Metal-Carbon bond-cleavage in "[Ru(1-2,5-eta-C_8H_{13})(CN-Xylyl)$_4$]PF_6 - The X-Ray Structure determination of [Ru2(CN-Xylyl)$_{10}$][BPH_4]$_2$** . Chalmers A.A, Liles D.C, Meintjies E, Oosthuizen H.E, Pretorius J.A, Singleton,E.
J. Chem. Soc.; Chem. Comm. (1985), ***19****, 1340-1341*

15 **The structure of Amorphous Sulfur** (The **λ**-phase of Sulfur)
Bruce E. Eichinger, Erich Wimmer & Jannie Pretorius. *MacroMol. Symp., (2001),****171****, 45-56.*

16 Schutte C.J.H. & Pretorius J.A. 2011. **A computational study of the molecular and crystal structure and selected physical properties of octahydridosilasequioxane–($Si_2O_3H_2$)$_4$. PART I**. Electronic and structural aspects. Proc. R. Soc. A 467:928-953 (Published online before print, October 27, 2010, doi:10.1098/rspa.2010.0388) -- **accepted**

17 Schutte C.J.H. & Pretorius J.A. 2011. **A computational study of the molecular and crystal structure and selected physical properties of octahydridosilasequioxane–(Si2O3H2)**4. **PART II**. Vibrational Analysis. Proc. R. Soc. A – submitted Aug, 2011 -- **accepted** Sept, 2011 (to be published online before print, October 2011)

18 ***A DFT study of the variation of the total molecular energy of the homologous zigzag polybenzenes with increasing number of rings***
C. J. H. Schutte, H.G. Miller, P.H. van Rooyen and J.A. Pretorius
Journal: ***Phys. Rev. Letters*** – *to be submitted*

Conference Papers

1. **Automation of a dated HILGER & WATTS X-ray Diffractometer. "Symposium on Automation in Chemistry**" – 1978, CSIR Conference Centre, South Africa. J.A.Pretorius
Also presented as a paper to MRC, Cambridge UK (group of **Prof. Uli Arndt**) to consider as a possible standard for the design of Area Detector X-ray units, to measure the single crystal status of high-pressure turbine blades.

2. **The intelligence of task-to-task communication during the online process computer simulation of chemical analysis** J.A.Pretorius.
Paper presented at the International Forum convened by the ICI-Laboratory Computing Panel. IBM Headquarters, WARWICK, UK, (1987). ***This theory and compute mechanism accepted as norm within ICI international (Europe, USA & SA) process control systems.***

3. **MOLECULAR WIRES**
Paper presented at the International Symposium on "Science of Minerals -- Derived Materials", J.A.Pretorius, (5-8 May, 1998), SA

4. **ISO-CYANURIC ACID as swimming pool water treatment agent (modeling study).**
Paper requested by an International (MONSANTO) court case, demanding the ban of this substance. Work undertaken in collaboration with **Prof. David Ollis'** group (Burmingham Univ., UK)
J.A.Pretorius, AECI: RN 52/B (1997).

5. **Adventures in Structural Research**
Paper presented at the 10th International Workshop on Materials Development (MaterialsDesign Inc.)
J.A.Pretorius, (6 Nov. 2008), TAOS, New Mexico, USA:
http://www.materialsdesign.com/users-group-meeting-2008

INTERNAL Papers (CSIR/ICI/AECI) – limited listing.

Theory and process application software for the AECI Coalefins Pilot Plant (1983)
J.A. Pretorius, AECI: AEQ 6.242/1/C, AEQ 6.242/2/C, Published as a joint venture with MOBIL, USA.
The first Methanol to Olefins (MTO) process plant in the world, utilizing a Zeolite catalyst

Computer Software for the effective migration of X-Ray diffraction Patterns to the BIOSYM modelling software environment. J.A.Pretorius, AECI: AEQ1 531/241/A
Undertaken as an International Consortium development with BIOSYM/MSI/Accelrys, USA

Proposed mechanism (modeling) and action of a Au-Cl promoted catalyst in the Hydrochlorination of Acetylene (PVC production). J.A.Pretorius, AECI: 1/2468/C (1997).
An alternative proposed to the international manufacturers for the polymerization of VCM, following the outcome **MENTHOL SYNTHESIS (Modeling)** of the legal case in the UK and restrictions placed on the use of Mercury as catalyst.

TBHQ (t-Butyl Hydroquinone) SYNTHESIS (modeling) J.A.Pretorius, AECI/ICI: RN (1996).

Research regulation-paper to obtain a product Quality Approval from FDA and FOODEX in opposition to Eastman Kodak, USA for the purpose as anti-oxidant in food products

A new novel catalytic route to the scaled synthesis of L-Menthol.
J.A.Pretorius, AECI/ICI: RN. (1997)
Research paper to design the plant and obtain an international product approval license from FDA, USA as Aroma Chemical

L-CARVONE SYNTHESIS (Molecular Modelling development of a novel reaction route)
J.A.Pretorius, AECI: RN 2265/B (1998).
Regulation paper to obtain an international production license from FDA, USA as Aroma Chemical
Work undertaken in collaboration with **Prof. Vladimir Hlavazek'** group (Buffalo Univ., USA)

Coalefins (Methanol to Olefins) process display/control and input parameter software development.
J.A.Pretorius, AECI: AEQ 6.246/C (1983).
JOINT VENTURE with MOBIL, USA and presented at Norsk Hydro (Norway), (1992).

Theory and control of a Carlo-Erba 1800 Sorptometer for Surface Area determination of process catalysts, **poly-ethylene process**-- J.A.Pretorius, Part A. AECI: AERD 1139/C (1983).

Proposed fibre optic Technical Computer Network, Modderfontein Factory (1988).
J.A.Pretorius, AECI: AEQ 1.531/122/B (1984).

Inline factory detonator statistics and database software design.
J.A.Pretorius, AECI: AEQ 6.280/A (1984).

Automation of a Philips PW1050/70 Xray Powder Diffractometer and Xray-Generator.
J.A.Pretorius, AECI: RN 0502/A (1987).

High-Level Network software, including mechanisms to access the ICI Computer Networks. J.A.Pretorius AECI: AEQ 1.531/190/A (1984).

Software Design to connect the Pinelands Computer Network to the 'INTERNET' Information Highway. J.A. Pretorius, AECI: RN 1918/A (1990).

Conformation and Configuration analysis on the molecular structure of an Organo-tin Complex --- in conjunction with Prof. Holzapfel (RAU). J.A.Pretorius, AECI: AEQ1 531/250/A (1995).

New procedure for the interactive computer modelling of Organo-metallic Compounds.
J.A. Pretorius, AECI: AEQ1 531/242/A (1996).

Software, theory and variable description of the STANJAN (Stanford Univ.) Thermodynamic Program.
J.A.Pretorius & V. Smithdorff, (1998), AECI: RN. Full recoding of the entire software program.

INTERNAL/SA Review Papers

BIO-DIESEL PROCESS DESIGN
Modeling of the full reaction mechanisms, including a new novel route for the catalytic trans-esterification of plant oil glycerides. Simultaneous separation of glycol and bio-diesel, formed in the same reaction kinetic cycle. Full online chemical Raman-analysis, control and interfacing with engineering cycles. J.A.Pretorius, Bhukka Engineering, Modderfontein (2005). PCM131-0005.

Optimization of the production of Ferric-sulphate as flocculent in water-purification processes. J.A.Pretorius, Bhukka Engineering, Modderfontein (2005)

COAL PROCESS PARTICLE SIZE CONTROL
Concept Engineering Package for the Measurement of Particle Size Distribution of Coal Delivery to the Gasification Plants at SASOL SYNFUELS, SECUNDA, (SASTECH).
J.A.Pretorius, E. v.Oudtshoorn, J. Kohler, Bhukka Engineering (May, 2006) PCM127-00-10-05-0007