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

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)