ICNTC E-CONFERENCE

INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

6th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

17 – 18 OCTOBER 2020

6th ICNTC PROCEEDINGS BOOK

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ICNTC E- Conference 2020

6th International Conference on New Trends in Chemistry

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Chemistry Department

Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of "**6th International Conference on New Trends in Chemistry**", to be held as based on Online Presentations dates between October 17-18, 2020

Conference was originally planned for April 2020 but due to the global spread of COVID-19 (Corona Virus) and The Council of Higher Education's declaration on "Measures to be Taken in Higher Education Institutions about COVID-19" (March 6, 2020) the conference is postponed to this **current date and will be organized based on online presentations.**

All informations are available in conference web site. For more information please do not hesitate to contact us. icnctcconference@gmail.com and info@icntcconference.com.

Limited number of oral and poster studies with the below mentioned topics will be accepted for our conference:

- Polymer Chemistry and Applications
- Pharmaceutical Chemsitry
- Computational Chemistry
- Bio Chemistry
- Physical Chemistry
- Analytical Chemistry
- Inorganic Chemistry
- Organic Chemistry
- Material Chemistry
- Environmental Chemistry

The most distinctive feature of ICNTC Conferences from other conference organizations is that the academicians working interdisciplinary can also attend to presentations performed in different speciality fields and they will also have the opportunity to meet with other academicians coming from various parts of the world.

Selected papers presented oral will be published in one of the Science Citation Index Expanded Journal.

We kindly wait for your attendance to our conference to be held on 16 –18th of October 2020,

Respectfully Yours,
On Behalf of the Organization Committee of ICNTC Conference
Assoc. Prof. Dr. Dolunay SAKAR DASDAN
6th ICNTC 2020 | Conference Chair
Yıldız Technical University – Istanbul / Turkey
Chemistry Department

SCIENTIFIC PROGRAM

17 OCTOBER 2020 SATURDAY

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08:50 – 09:00
Welcome Speech : **Assoc. Prof. Dr. Dolunay SAKAR DASDAN /** Conference Chair
Yildiz Technical University, Turkey

09:00 – 09:40
Keynote Speaker : **Assoc. Prof. Dr. Sameh BOUDIBA** / Tebessa University, Algeria
Speech Title :Anthracene Based Conjugated Polymers for Optoelectronic Applications

09:40 – 09:45	**B R E AK**

SESSION A

SESSION CHAIR	**Assoc. Prof. Dr. Dolunay SAKAR DASDAN** Yildiz Technical University	
TIME	**PAPER TITLE**	**PRESENTER** / CO AUTHOR
09:45– 10:00	Effect of Incorporation of Zinc Oxide on the Properties of PHBV	**Semra KIRBOGA**
10:00– 10:15	Green synthesis of ZnO particles and their application as catalysts in the transesterification of methyl benzoates	**Mohamed Soliman,** Elisabete Alegria, Ana Ribeiro, Marta Alves, Fátima Montemor and Armando Pombeiro
10:15– 10:30	Antibacterial Activity and Physical Properties of Bovine Gelatıne-Chitosan Wound Dressing Films Supplemented With Propolis	**Ilknur KUCUK**, Nigar YILDIRIM
10:30– 10:45	The Effects of Additives on Particle Size and Morphology of Barium Sulfate Crystals	Egemen OYMAN, **Emel AKYOL**
10:45– 11:00	Computational Examination of Degradation Reactions of Precious Endocrine Disruptors Molecules Through Surface Water	**Simal KURUMOGLU**, Yelda YALCIN GURKAN
11:00– 11:15	Molecular Sensors: Design, Synthesis and Practical Applications	**Erman KARAKUS**
11:15– 11:30	Theoretical and Molecular Docking Analysis of Silver-nhc Complexes as a Potential Anticancer Agent	**Neslihan SAHIN**, Elvan USTUN
11:30– 11:45	Structure of Drug-Polymer Composites Prepared by Nano Spray Dryer	**Mirella MIRANKO**, Laszlo TRIF, Judit TOTH, Tivadar FECZKO
11:45- 12:00	Polymorphism and Topochemical Reactivity in	**Fabio BORBONE** , Roberto

	Fusedring Heteroaromatics	CENTORE , Emmanuele PARIS , Antonio CARELLA

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SESSION B

SESSION CHAIR	**Prof.Dr.Sevil YUCEL** Yildiz Technical University	
TIME	**PAPER TITLE**	**PRESENTER** / CO AUTHOR
13:00-13:15	Biodegradable Zwitterionic Nanoparticles With a Biologically Relevant Ucst at Physiological Salt Concentration	**Mattia SPONCHIONI**, Umberto CAPASSO PALMIERO, Davide MOSCATELLI
13:15 – 13:30	New Voltammetric Method for Determination and Electrochemical Behaviors of Oxaliplatin by cpt-bdd Electrode	**Mehmet ASLAN**, Abdulkadir LEVENT
13:30 – 13:45	Synthesis of Poly (Methyl Vinyl Ether-Co-Maleic Anhydride)-Cu+2-Bovine Serum Albumin Biocomplex and Investigation of Different pHs and Salt Concentration Effects on The Stability of Poly (Methyl Vinyl Ether-Co-Maleic Anhydride)-Cu+2-Bovine Serum Albumin Biocomplex in Aquous Solutions	Rahime Bilge BORKLU, **Dolunay SAKAR DASDAN,** Mesut KARAHAN
13:45 – 14:00	Development of Nanostructured-Graphene-Supported Silver Nanoparticles as Catalysts for Electroreduction of Oxygen in Alkaline Electrolyte	**Sylwia ZOLADEK**, Magdalena BLICHARSKA-SOBOLEWSKA, Agnieszka ZLOTOROWICZ, Iwona Agnieszka RUTKOWSKA, Krzysztof MIECZNIKOWSKI, Enrico NEGRO, Vito DI NOTO, Pawel KULESZA
14:00 – 14:15	Preparation and Co2 Permeabilities of Peba Mixed Matrix Membranes With Metal Organic Frameworks	**Nagehan CELIK**, Sennur DENİZ
14:15 – 14:30	Novel Electrochemical Biosensing of Tyramine Based on Fe_2o_3 NPs-Multiwall Carbon Nanotubes-Hexaamminerutheniıum-Chitosan Modified Glassy Carbon Electrode	**Berna DALKIRAN**
14:30-14:45	Stabilization and Harvesting of Hesperetin Microrods From the Hesperetin Stabilised Via Plantacare 2000 Solution by Using Template-Assisted Particle Infiltration Method	**Yesim KARAHAN**, Marcel POURASGHAR, Marc SCHNEIDER, Cornelia M. KECK, Dolunay SAKAR DASDAN
14:45– 15:00	One Pot Synthesis of Piperidine Derivatives and Evaluation of Their Anticancer Potential	**Zulfiqar Ali KHAN**

15:00-15:15	**B R E AK**

17 OCTOBER 2020 SATURDAY

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SESSION C

SESSION CHAIR	**Mattia SPONCHIONI** Politecnico di Milano	
TIME	**PAPER TITLE**	**PRESENTER** / CO AUTHOR
15:15– 15:30	Optimization of Drying Process for Green Bricks Using Response Surface Methodology	**Bercem KIRAN YILDIRIM**, Ebru MANCUHAN, Sibel TITIZ SARGUT
15:30– 15:45	Water Quality in the Armutlu Beach	**Esin BOZKURT KOPUZ**
15:45– 16:00	New Voltammetric Strategy for Determination and Electrochemical Behaviors of Metformin by Pencil Graphite Electrode	**Yalcin ALTUNKAYNAK**, Omer YAVUZ, Abdulkadir LEVENT
16:00– 16:15	Facile Access to O-Heterocycles Using N-Methyl-1-(Methylthio)-2-Nitroethenamine (NMSM)	**Musawwer KHAN**, Saigal and Sumbulunnesa SHAREEF
16:15– 16:30	Bodipy Functionalized Molecular Metal Oxides: Synthesis, Characterization and Properties	**Seda CETINDERE**
16:30– 16:45	Antiproliferative Silver-NHC Complexes: Structural and Global Reactivity Descriptor Analysis and Molecular Docking Study	**Elvan USTUN**, Neslihan SAHIN
16:45- 17:00	Thermal and Mechanical Properties of Continuous Glass Fiber/Pet Composites	**Melis Eldem HEPER**, Sennur DENİZ
17:00- 17:15	Iridium Oxide İmmobilized On Cerium Oxide For Enhanced Water Oxidation	**Kadriye Özlem HAMALOĞLU,** Rukiye BABACAN TOSUN, Ali TUNCEL
17:15-17:30	Temperature Control In Polystrene Polymerization Reactor By Using Neural Network Model Predictive Algorithm	Erkin ETIKE, **Gülay ÖZKAN,** Hale HAPOĞLU

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POSTER SESSION A

SESSION CHAIR	**Prof. Dr. Mustafa GAZI** Eastern Mediterranean University **Assoc. Prof. Dr. Yelda YALCIN GURKAN** Namik Kemal University **Assoc. Prof. Dr. Elvan ÜSTÜN** Ordu University	**5 min oral presentation after that questions from participants**
TIME	**PAPER TITLE**	**PRESENTER** / CO AUTHOR
17:30-18:30	Effect Of N-Butanolic Extract Of A Plant Growing Spontanusely In Central Algeria As An Additive In Electrodeposition	**Karima HANINI1**, Sameh BOUDIBA, Merzoug BENAHMED, Hocine LAOUER and Louiza BOUDIBA
	Electrochemical Oxidation of Vildagliptin on Pencil Graphite Electrode: Extremely Sensitive Determination in Drugs and Human Urine With Square Wave Voltammetry	**Yalcin ALTUNKAYNAK**, Omer YAVUZ, Abdulkadir LEVENT
	Computational Examination of Degradation Reactions of Butralin	**Simal KURUMOGLU**, Yelda YALCIN GURKAN
	The Properties of Phbv/Caco3 Composites Prepared by Melt Processing	**Semra KIRBOGA**, Mualla ONER
	Determination of Hexanal as Marker of Lipid Oxidation in Edible Oils by Headspace Gas Chromatography	**Birute BUGELYTE**, Gintare PIPIRAITE, Vilius POSKUS, Vida VICKACKAITE
	Synthesis and Characterisation of a Glutathıone-Stransferase (Hgstp1-1) Single NUCLEOTIDE Polymorph	**Sadhna MATHURA**
	Investigation of Structural and Magnetic Properties of Nickel Doped Iron Oxide Nanoparticles Depending on the Amount of Dope Values	**Nurcan DOGAN**, Namik DIKTAŞ, Ceren ERSEN , Ayhan BINGOLBALI
	Analysis of Molecular Orbital Energies, Global Reactivity Descriptors, and Electronic Transitions of [Mn(CO)3(bpy)(N-benzimidazole)]PF6] Complex by DFT/TDDFT-Based Computational Methods	**Dolunay ŞAKAR DAŞDAN,** Elvan ÜSTÜN
	Bitter Vetch Seed Oil (Vicia Ervilia L.) – A New Source of Bioactive Components	**Zhana PETKOVA**, Ginka ANTOVA, Olga TENEVA, Maria ANGELOVA-ROMOVA
	Different Response of A 2-Ureido-4-Ferrocenyl Pyrimidine Sensor to CF_3SO_3H and CF_3CO_2H Guests	**Soma J. KESZEI**, Szabolcs BALOGH , Csaba FEHER , Lívia NAGY , Nikolay TUMANOV, Johan WOUTERS, Gyorgy LENDVAY ,Rita SKODA-FOLDES

18 OCTOBER 2020 SUNDAY

09:00 – 09:30
Invited Speaker : **Prof. Dr. Mustafa GAZI** / Eastern Mediterranean University – North Cyprus
Speech Title : Chitosan Based Adsorbents for Boron Removal from Aqueous Solutions

SESSION D

SESSION CHAIR	**Prof. Dr. Huriye ICIL** Eastern Mediterranean University	
TIME	**PAPER TITLE**	**PRESENTER** / CO AUTHOR
09:30– 09:45	Polyphosphazene Based Fuel Cell Membranes	**Elif Busra CELEBI**, Ferda HACIVELIOGLU
09:45– 10:00	Zn-Chitosan Nanoparticles as Ecofriendly Priming Agent: Re-Modulate Antioxidant Potential and Biochemical Attributes in Wheat Seeds for Sustainable Productivity	Hameed ARRUJE, Khalid ALVINA, Hameed AMJAD, Ahmed TOHEED, **Farooq TAHIR**
10:00- 10:15	Mechanical Properties of Biodegrarable PLA/PCl Blend Films Prepared With A-Tocopherolf	**Nudem DENIZ**, Sennur DENIZ
10:15– 10:30	Synthesis and Alpha-Glucosidase Inhibition Studies of 1,2-Benzothiazine Derivatives	**Matloob AHMAD**
10:30– 10:45	Sodium Nitroprusside Mediated Priming Memory Invokes Water-Deficit Stress Acclimation in Wheat Plants Through Physio-Biochemical Alterations	**Hameed ARRUJE**, Farooq TAHIR, Hameed,Amjad Sheikh Munir AHMAD
10:45– 11:00	Antimony Adsorption Study of Chitosan Produced From Caridea and Brachyura Shells	**Zehra Ozden OZYALCIN**, Azmi Seyhun KIPCAK
11:00– 11:15	Processability Improvement of Natural Rubber in Mastication Step by Residual Carbon Black Addition	**Merve PEHLIVAN**, Bora ATALIK, Sezgin GOKCESULAR
11:15– 11:30	Susceptibility of 99mtc-Ciprofloxacin for Common Infection Causing Bacterial Strains Isolated from Clinical Samples: An in Vitro and in Vivo Study	**Syed Ali Raza NAQVI**, Aysha AZIZ, Hassina SABIR

11:30 – 11:45	**B R E AK**

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SESSION E

SESSION CHAIR	**Assist.Prof.Dr.Sennur Deniz** Yildiz Technical University	
TIME	**PAPER TITLE**	**PRESENTER** / CO AUTHOR
11:45- 12:00	A Computational Study on the Structural and Spectral Properties of 2-Hydroxy-4-(2-Hydroxyethoxy)-2-Methylpropiophenone	**Asim MANSHA**, Noreen AKRAM, Sadia ASIM
12:00– 12:15	Production of Biocomposite Tissue Scaffolds by Using Boron-Containing Bioactıve Glass and Collagen/Gelatin Hybrid Polymer for Bone Tissue Engineering	**Eda GUNEY**, Ceren KECECILER, Dilan ALTAN, Sevil YUCEL
12:15– 12:30	Novel N-4-Piperazinyl-Ciprofloxacin-Aniline Hybrids: Synthesis and in Vitro Biological Evaluation as Anticancer Agents	Rabia AKHTAR, **Ameer Fawad ZAHOOR**, Azhar RASUL, Matloob AHMAD, Muhammad Naveed ANJUM, Muhammad AJMAL and Zohaib RAZA
12:30- 12:45	A Novel Nanozyme for Colorimetric Detection Of L-Histidine	**Duygu YILDIRIM**, Cigdem KIP, Ali TUNCEL
12:45- 13:00	Optical Molecular Imaging: Fluorescent Smart Probes for Pathogen Detection	**Muhammed UCUNCU**

13:00 – 13:45	**LUNCH BREAK**

SESSION F

SESSION CHAIR	**Prof. Dr. Mustafa GAZI** Eastern Mediterranean University	
TIME	**PAPER TITLE**	**PRESENTER** / CO AUTHOR
13:45– 14:00	Cyclodextrin-Calixarene Nanosponges for the Adsorption of Lead Ion From Aqueous Solution	**Salvatore CATALDO**, Alberto PETTIGNANO, Paolo Lo MEO, Demetrio MILEA
14:00– 14:15	Catalyic Effect of Amines on a Co2bol Absorption Performance	**Ozge YUKSEL ORHAN**
14:15– 14:30	Experimental and Theoretical Analysis of a Refrigeration System With Phase Change Material (PCM) Integration	**Tugce NOYA**, Bercem KIRAN YILDIRIM, Ebru MANCUHAN, Sibel TITIZ SARGUT
14:30– 14:45	Synthesis, Characterization and Structure of Chlorido Platinum(Iı) Saccharinate Complex Bearıng 1,1-Bis(Diphenylphosphino) Methane	**Ceyda ICSEL**
14:45– 15:00	Application Of Bismuth Film Electrode in Determination Of Loratadine by Cathodic Stripping Voltammetry in the Presence of Cationic	**Gunay ONAL**, Yalcin ALTUNKAYNAK, Abdulkadir LEVENT

	Surfactant	
15:00- 15:15	Effect of Temperature and Reaction Time on Structural, Morphological and Magnetic Properties of zn-doped fe_3o_4 Nanoparticles ($Zn_{0.25}Fe_{2.75}O_4$) Synthesized by the Hydrothermal Method	**Nurcan DOGAN**, Gulsum CALISKAN

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15:15 – 15:45
Invited Speaker **: Prof. Dr. Huriye ICIL /** Eastern Mediterranean University – North Cyprus
Speech Title **:** Novel Bay-Substituted Perylene Bisimides

15:45 - 16:00	**B R E AK**

SESSION G

SESSION CHAIR	**Prof.Dr.Nursen SARI** Gazi University	
TIME	**PAPER TITLE**	**PRESENTER /** CO AUTHOR
16:00- 16:15	Production of Novel Composite Films Based on Pva-Biosilica	Enver Can KILIC, Emel AKYOL, Burcu KARAKUZU IKIZLER, Ali Can OZARSLAN, **Sevil YUCEL**
16:15– 16:30	A Facile Method to Prepare Bismuth Doped Zno Photocatalysts and Their Photocatalytic Property	**Nazli TURKTEN**
16:30– 16:45	Chemical Reaction in Powder Mixtures of Calcium Hydroxyapatite and Potassium Hydrosulfate Under Mechanical Activation in Acetone Medium	**Tatiana SAFRONOVA**, Marat AKHMEDOV, Tatiana SHATALOVA,Snezhana TIKHONOVA, Gilyana KAZAKOVA
16:45– 17:00	A Computational Study Of 2,3-Dihydrospiro[Carbazole-1,2'-[1,3]Dithiolan]-4(9H)-One Compound: Structure, FT-IR, NMR, NLO, and NBO Analyses	**Goncagul SERDAROGLU,** Nesimi UlLUDAG
17:00– 17:15	The Hydrolysis of Tert-Butylamine Borane By Using Ni-Zr-B Catalyst for Hydrogen Production	**Hatice Begum MURATHAN**, Goksel OZKAN
17:15 – 17:30	Rh-Based Ternary Catalyst for the Catalytic Dehydrogenation of Hydrazine Borane as an Chemical Hydrogen Storage Material	**Merve Rabia GURLUK**, Gülay OZKAN, Goksel OZKAN
17:30– 17:45	New Triazolo-Triazole Derivatives: Redox and Emission Properties and Cu(I1) Complexes	**Sandra FUSCO** , Emmanuele PARISI , Sabato VOLINO , Carla MANFREDI , Roberto CENTORE

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POSTER SESSION B

SESSION CHAIR	**Prof. Dr. Huriye ICIL** Eastern Mediterranean University **Dr. Emel Akyol** Yıldız Technical University **Assoc. Prof. Dr. Nurcan DOGAN** ildiz Technical University	**5 min oral presentation after that questions from participants**
TIME	**PAPER TITLE**	**PRESENTER** / CO AUTHOR
17:45-18:45	A Spectrophotometric Investigation of the Interaction Between DNA and the Anticancer Drug Candidate Schiff Bases and Their Pt (II) Complexes	Elvan HASANOGLU OZKAN, Suheyla Pinar CELIK, Leyla ACIK, Ali DISLI, **Nursen SARI**
	Interactions of New Tetrazolato Complexes Containing VIII B Group Transition Metals With DNA	**Elvan HASANOGLU OZKAN**, Suheyla CELIK, Leyla ACIK, Ali DISLI, Nursen SARI
	The Contribution of Electronegative Groups on The Synthesis and the Antimicrobial Effects of Tetrazol Compounds Containing Different Substitutent Groups	**Elvan HASANOGLU OZKAN**, Hatice OGUTCU, Ali DISLI, Nursen SARI
	Effect of Mixer Rotor Wing Types on Compound Properties	**Merve PEHLIVAN,** Bora ATALIK, Sezgin GOKCESULAR
	The Effects of Naphthenic Oil, BR, NR and Content of Vinyl in S-SBR on Passenger Tread Compounds	**Duygu KABAKOGLU**, Sezgin GOKCESULAR
	Electroanalytical Determination of Progesterone Hormone Using Boron-Doped Diamond Electrode	**Muhlis UCAR**, Abdulkadir LEVENT
	Synthesis of 16α-Substituted-Pregnenolone Derivatives Via Ionic Liquid-Catalyzed Aza-Michael and Thio-Michael Addition	**Lilla MAKSO**, Rita SKODA-FOLDES
	Investigation of Switchable Polarity Solvents and Their Application in Claisen-Schmidt Reaction of Steroids	**David ISPAN**, Rita SKODA-FOLDES
	Aminocarbonylation in the Presence Of Supported Palladium Catalyst	**Eniko Nagy**, Bernadett ADAMCSIK, Mate PAPP, Bela URBAN, Rita SKODA-FOLDES
	CO_2 MethanatİOn WİTh Ce Promoted Ni Catalyst Supported on Mixed Materials of Al_2O_3 and Y_2O_3	**Nyamsuren BATTUMUR**, Enkhsaruul BYAMBAJAV

	Antioxidant Activity of New Glycoconjugates Containing Selenium	**Luigia SERPICO**, Mauro De NISCO, Flavio CERMOLA, Michele MANFRA, Claus JACOB, Silvana PEDATELLA
	Preparation of Calcium Polyphosphate Powder Containing Amorphous Carbon	**Tatiana SAFRONOVA**, Yanis PAIANIDI, Tatiana SHATALOVA, Yaroslav FILIPPOV, Gilyana KAZAKOVA, Umarali UMIROV, Otabek TOSHEV
	Synthesis And Characterızatıon Of Phosphazene-Based Epoxy Bınders	**Elif Busra CELEBI**, Halil DUYAR, Cengiz AYAR Rumeysa BARAN, Ferda HACIVELIOGLU
	Tetra 7-Oxy-4-(Pyrıdın-3-Yl)Coumarin Substituted Copper (Iı) and Cobalt (Iı) Phthalocyanines: Synthesis, Spectroscopic Properties and Theoretical Study	**Yelda YALCIN GURKAN**, Simal KURUMOGLU, Caner Yahya BOYAR, Yasemin KESKEK KARABULUT, Meryem CAMUR

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SYNTHESIS AND CHARACTERISATION OF A GLUTATHIONE-*S*-TRANSFERASE SINGLE NUCLEOTIDE POLYMORPH

Sadhna MATHURA

Faculty of Science, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa.
sadhna.mathura@wits.ac.za

Abstract

Glutathione-S-transferases (GST) comprise a superfamily of multifunctional enzymes involved in catalytic cellular detoxification reactions. In this work we aimed to investigate the structural and functional properties of a single nucleotide polymorph (P124A) in the hydrophobic domain of canonical cytosolic human GST class pi (hGSTP1-1), relative to wildtype. Our strategy was to first synthesize the P124A mutant by site-directed mutagenesis. Secondly, we overexpressed and purified the mutant enzyme. We then structurally characterized the enzyme using spectroscopic methods. Lastly, the P124A mutant enzyme was functionally characterized to examine how the position of this mutation influenced the catalytic and stability properties at the binding sites. Circular dichroism and fluorescence spectra reveal minor secondary and tertiary alterations of P124A structure relative to wildtype. CDNB assay revealed minor alterations in catalytic activity relative to wildtype.

Key Words: *hGSTP1-1; SNP; polymorphism; structure-function relationship; detoxification proteins.*

1. Introduction

Glutathione-S-transferases (GSTs, E.C. 2.5.1.18) comprise a superfamily of multifunctional enzymes involved in catalytic cellular detoxification reactions [1]. They are widely distributed in pro- and eukaryotic systems alike. In eukaryotic systems, GST proteins can be found in a variety of organs including liver, kidneys and the brain. Within the cell, GST proteins are distributed in organelles as well as in the cytoplasm [1].

As classical phase II detoxification enzymes, GSTs play a critical role in protecting the cell against oxidative stress and in the detoxification of toxic foreign chemicals. Their function is the intracellular detoxification of xenobiotics by catalyzing the covalent binding of reduced glutathione (GSH) onto nonpolar xenobiotic molecules through a nucleophilic attack mechanism. GST binds GSH and initiates the deprotonation of the sulfhydryl group. The reduced glutathione-GST complex then binds to the xenobiotic substrate. The metabolized xenobiotics are then expelled through the mercapturate pathway [2-3].

There is growing evidence linking GSTs to human health and well-being [4]. Mutations in GST enzymes, specifically single nucleotide polymorphisms (SNP), have been linked to several human diseases and ailments [3-6]. Elucidating GSTs complex structure-function relationships has therefore garnered much research interest. As such, this work focuses on the structure and function of canonical cytosolic human GST class pi (hGSTP1-1) by examining an SNP mutation at the dimer-dimer interface, P124A. The key question being, what effects does this single nucleotide mutation have on its structure, stability and catalytic function?

hGSTP1-1 is homodimeric (Fig. 1). Each monomer (subunit) comprises two distinct domains; each domain within a subunit containing a ligand-binding site. Firstly, a GSH-specific G-site is contained within the smaller N-terminal thioredoxin-like domain. Secondly, a non-specific hydrophobic substrate-binding H-site is contained within the larger all-helical C-terminal domain [7]. P124A is found at the subunit interface within the C-terminal domain.

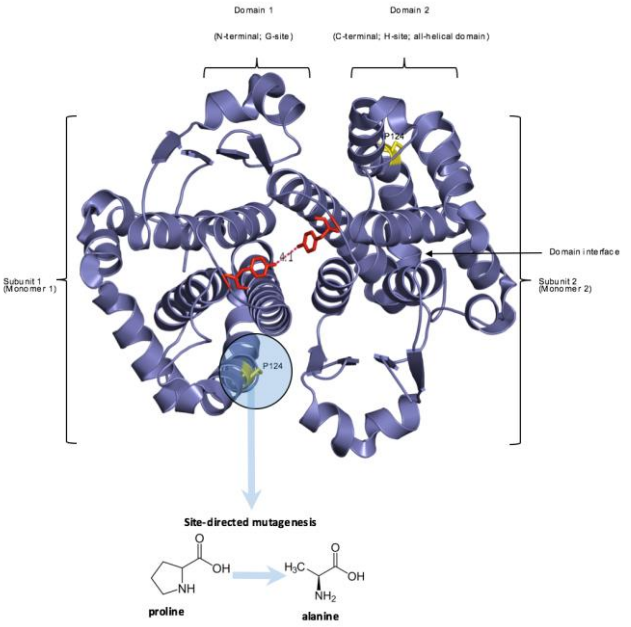

Fig. 1. Quaternary structure of the homodimeric hGSTP1-1 [8]. The highlighted region indicates the P124A mutant.

2. Experimental

2.1 Mutagenesis, transformation and sequencing of mutant P124A [9-10]

Plasmid DNA encoding the hGSTP1-1 mutant, P124A was synthesized using site-directed mutagenesis kit QuikChange^{TM} (Stratagene, CA). Oligonucleotide primers for the mutagenesis were designed (Primer-X software; http://bioinformatics.org/primerx). Plasmid DNA was sequenced (Inqaba Biotechnical Industries (Pty) Ltd, Pretoria, South Africa) and aligned using BLAST (https://blast.ncbi.nlm.nih.gov/Blast.cgi) and 4Peaks software (https://nucleobytes.com). Plasmids were then transformed into E. coli T7 cells for overexpression of the P124A mutant enzyme.

2.2 Overexpression and purification mutant P124A using standard methods [10]

Mutant enzyme overexpression was induced using an IPTG (0.2 mM; 30°C; 8hrs). The cultured cells were harvested by centrifugation, re-suspended (50 mM Tris-HCl buffer, pH 8.0; -20 °C). Purification was achieved using cobalt HisTrap™ column with binding buffer [50 mM Tris-HCl pH 8.0, 0.5 M NaCl, 50 mM imidazole (eluted with 300 mM), 0.02 % sodium azide], and analysed using SDS-PAGE.

2.3 Structural characterization of mutant P124A using standard methods [10]

Both far-UV circular dichroism (CD) and fluorescence emission spectra measurements were conducted with 1 µM of both wildtype and P124A enzymes in phosphate buffer (pH 7.4, 20 mM, 20 ^{o}C).

2.4 Functional characterization of mutant P124A using standard methods [10]

The enzyme-catalysed conjugation of CDNB to GSH was monitored spectroscopically by measuring the formation of 1-(S-glutathionyl)-2,4-dinitrobenzene at 340 nm. At at 20 °C, samples of protein were prepared (1–10 nM, 100 mM phosphate buffer; pH 7.5, 1 mM GSH). The conjugation reaction was initiated by the addition of a 30 mM stock solution of CDNB to create a final assay CDNB

concentration of 1 mM and a final assay volume of 3 ml. The reaction was monitored at 340 nm (1 min; 20 °C).

3. Results and Discussion

3.1 Synthesis data: primer design, sequencing and alignment, SDS-PAGE gel

The hGSTP1-1 mutant P124A was synthesized in order to investigate the structure-function relationship of the wildtype hGSTP1-1. Both forward and reverse primers were successfully designed for the proline to alanine point mutation (Fig 2A). Sequencing data indicates the mutant codon for alanine and the subsequent alignment of mutant vs wildtype protein (Fig 2B). The truncated sequence alignment for hGSTP1-1 P124A indicates 99% alignment with known hGSTP1-1 wildtype protein (Fig 2A). The overexpressed mutant protein was purified and analyzed using SDS-PAGE gel analysis; single band indicating high purity mutant protein (Fig 2C).

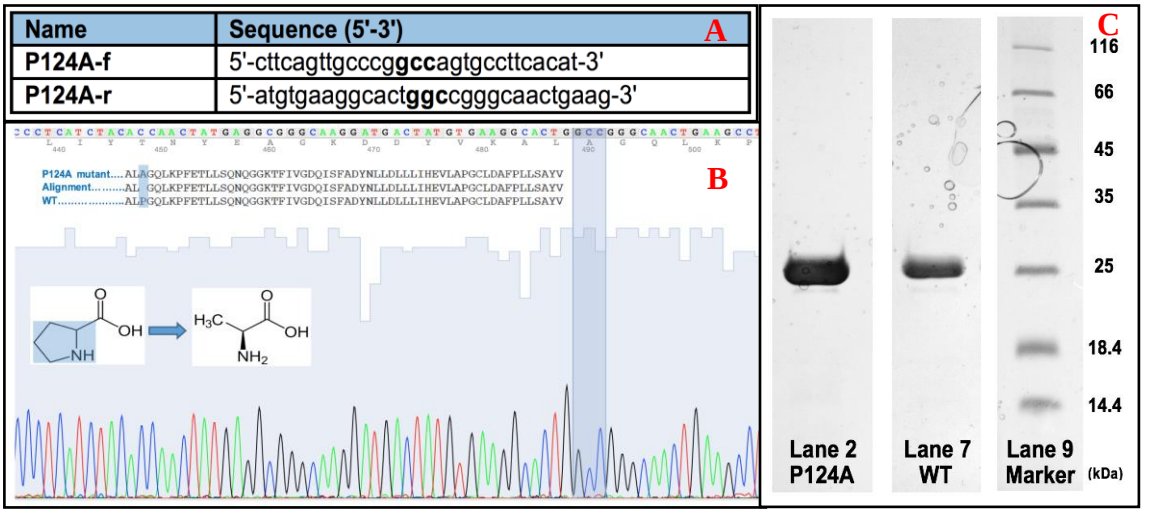

Fig. 2. Synthesis data: (A) forward and reverse priers used for site-direct mutagenesis of hGSTP1-1 P124A mutant. (B) truncated sequence alignment for mutant hGSTP1-1 P124A yielding 99% identity with known PDB data bank indicating the point mutation [8]. (C) SDS-PAGE analysis of wildtype (Lane 7) and mutant P124 A (Lane 2) in 16% acrylamine; glycine; 120 V;

3.2 Characterization data: structural and functional analysis

A summary of the synthesis and characterization data is tabulated for hGSTP1-1 wildtype and P124A mutant (Table 1). Synthesis data are tabulated for the number of colonies grown on agar plates. Findings revealed that there is a significant difference between the approximate number of colonies produced between the mutant and the wildtype. Following this trend, the overexpression of the mutant protein requires milder incubation conditions than wildtype in order to prevent protein aggregation. Additionally, P124A consistently expressed relatively lower concentrations of active protein as compared to wildtype, on a batch by batch basis. Estimated mass (in kDa) were determined using SDS-PAGE analysis and found to be approximately 25 kDa for both wildtype and for P124A subunits, respectively.

Structural data revealed only minor conformational changes in P124A relative to wildtype. UV-vis spectra indicated that maxima were approximately 282 nm with a minor increase in the intensity for P124 relative to wildtype. Intrinsic fluorescence showed maximum excitation at 340 nm and 342 nm for both proteins, with a minor increase in intensity in P124A. Far-UV CD showed spectra that were consistent with hGSTP1-1 with peaks at 190 nm, 208 nm, 222 nm.

Functional data (CDNB analysis and thermal unfolding) showed a minor decrease in activity and stability in P124A as compared to wildtype.

Table 1. Summary of synthesis and structural data for the comparison of hGSTP1-1 wildtype and mutant P124A

		hGSTP1-1 WILDTYPE	**hGSTP1-1 MUTANT P124A**
Synthesis data	Number of colonies	~ 10 colonies per cm^2	~ 04 colonies per cm^2
	Overexpression (Incubation conditions)	3hrs, 37 ^oC, 100 µ g /mL ampicillin	8hrs, 30 ^oC, 50 µ g /mL ampicillin
	Concentration[1]	~ 30 mg/mL	~ 25 mg/mL
	Estimated protein mass[2]	25 kDa	25 kDa
Structural data	Amino acid distance[3]	P124-P124 ~ 37 Å	A124-A124 ~ 38 Å
	UV-Vis maxima	282 nm	283 nm (increased intensity)
	Intrinsic fluorescence	Excitation 280 nm → 340 nm Excitation 295 nm → 342 nm	Excitation 280 nm → 340 nm Excitation 295 nm → 342 nm (increased intensity)
	Far-UV CD	Peaks: 190 nm, 208 nm, 222 nm	Peaks: 190 nm, 208 nm, 222 nm (increased intensity)
Functional data	Specific activity	43.9 ± 1.6 µ.mol.min^{-1}.mg^{-1}	42.5 ± 1.1 µ.mol.min^{-1}.mg^{-1}
	Thermal denaturation	$T_m = 55 \pm 3$ ^oC	$T_m = 51 \pm 3$ ^oC

1. estimated using Beer's Law and NanoDrop© instrumentation
2. estimated using SDS-PAGE analysis; mass per monomer subunit
3. estimated using Pymol simulations

4. Conclusions and Future Work

An SNP mutant in hGSTP1-1, P124A, was investigated in terms of structure and function. These were then compared to the wildtype, hGSTP1-1. Our findings at this preliminary stage revealed no significant difference in secondary and tertiary structure between P124A and wildtype. The CDNB enzymatic activity was not significantly different. Future work would be to compare the solid-state chemistry by protein crystallization of P124A and wildtype.

5. Acknowledgements

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6. References

[1] Vasieva, O.; *Current Molecular Medicine*, 2011, **11**, 129-130.

[2] Sheehan, D.; Meade, G.; Foley, V. M.; Dowd, C. A.; *Biochem. J*., 2001, **360**(1); 1-16.

[3] Armstrong, R. N.; *Chemical Research in Toxicology*, 1997; **10**(1); 2–18.

[4] Tew, K. D.; Manevich, Y.; Grek, C.; Xiong, Y.; Uys, J.; Townsend, D. M.; *Free Rad. Biol. And Med*., 2011, **51**(2); 299-313.

[5] McIlwain, CC; Townsend, DM and Tew, KD; *Oncogene*, 2006, **25**, 1639-1648.

[6] Hayes, J. D.; Strange, R. C.; *Pharmacology*, 2000, **61**, 154-166.

[7] Hezagyt, U.M., Mannervik, B., Stenberg, G.; *J. Biol. Chem*., 2003, **279**, 9586-9596.

[8] hGSTP1-1 structure from protein data bank (PDB ID: 2a2r): http://www.rcsb.org/pdb/

[9] SNP database (https://www.ncbi.nlm.nih.gov/snp/)

[10] Molaudzi, Z., Structural and functional analysis of peroxiredoxin 6 and glutathione transferase P1-1, University of the Witwatersrand, Johannesburg, South Africa, dissertation, 2017.

CO_2 METHANATION WITH Ce PROMOTED Ni CATALYST SUPPORTED ON MIXED MATERIALS OF Al_2O_3 AND Y_2O_3

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Abstract
The activity of the 15%Ni catalyst supported on γ-Al_2O_3, the 15%Ni catalysts supported on a mixture of γ-Al_2O_3 and Y_2O_3 (Ni/Al-yY; y=5, 15, or 25 wt%) and the Ce promoted Ni catalysts supported on the mixture of γ-Al_2O_3 and Y_2O_3 (Ni-xCe/Al-yY; x=1, 2, or 5 wt% and y=15 wt%) were investigated for CO_2 methanation. Reactions were performed at the temperature of 350 ˚C in the ambient pressure of H_2:CO_2=4:1 feed gas with the GHSV of 3000 h^{-1}. The addition of Y_2O_3 in the main support material improved the distribution of nickel catalyst, consequently increased the activity of CO_2 methanation. However, the most convenient content of the Y_2O_3 additive in Ni/Al-yY was 15 wt%. Then, an effect of Ce promoter on Ni-xCe/Al-15Y was investigated for CO_2 methanation. It was concluded that the Ni-2Ce/Al-15Y catalyst gave the highest CO_2 conversion of 92.5% and the largest CH_4 yield of 92.2% at the present reaction conditions.

Key words: *CO_2 hydrogenation; Ceria, Al_2O_3-Y_2O_3 combined support; promoter*

1. Introduction

The process of producing methane gas by CO_2 hydrogenation is an environmentally friendly and highly efficient technology that can be applied in clean and renewable energy sector [1-2]. Recently, it was reported that the presence of 2.5-10 wt% CeO_2 on a 10 wt% Ni/γ-Al_2O_3 catalyst, which was prepared by the ultrasonic incipient impregnation method, exhibited highly improved catalytic activity compared to the unpromoted Ni/γ-Al_2O_3 catalyst [1]. In another study, the 0.25-6.00 wt% CeO_2 promoted Ni/Al_2O_3 catalysts prepared by co-impregnating method could improve the CO_2 methanation activity because the addition of CeO_2 alters the interaction between Ni and Al_2O_3, and improves the reducibility of the catalyst [2].

The influence of the cerium promoter has not been reported in the case of a combination of γ-Al_2O_3 and Y_2O_3 supports for the Ni catalyst development in CO_2 methanation. Our work aimed to study the effects of the contents of Ce promoter and Y_2O_3 support additive on the catalytic performance of CO_2 methanation over Ni-xCe/Al-yY catalysts.

2. Experimental

Catalyst preparation. In a every run, 10 g of catalyst was prepared. The nominal content of metal was 15 wt%. Ni-xCe/Al-yY catalysts were prepared by the impregnation-co-precipitation method and the procedure applied was as follows: (I) For preparation of the catalyst without support additives, appropriate quantities of γ-Al_2O_3 were dissolved in distilled water, followed by stirring at 80 ˚C for 30 min. (II) In case of combined supports, yY_2O_3 (y=5,15, or 25 wt%) to the main support solution of γ-Al_2O_3 were added. To this solution, stoichiometric quantities of $Ni(NO_3)_2{\cdot}6H_2O$ and Na_2CO_3 were simultaneously added dropwise at 80 ˚C for 1 h to give a precipitate of $Ni(CO_3)$. Then, the mixture was cooled to ambient temperature. The precipitate was filtered, and washed by distilled water. The obtained samples were dried at 110 ˚C for 12 h and calcined at 500 ˚C for 4 h. The prepared catalyst was defined as Ni/Al, Ni/Al-5Y, Ni/Al-15Y, and Ni/Al-25Y, respectively. (III) Then, the Ce-promoted Ni-xCe/Al-15Y (x=1, 2, or 5 wt%) catalysts were also prepared by the impregnation-co-precipitation method with the same procedure as above. $Ce(NO_3)_3{\cdot}6H_2O$ was used as a precursor of cerium. Three samples were denoted as follows: Ni-1Ce/Al-15Y, Ni-2Ce/Al-15Y, and Ni-5Ce/Al-15Y.

Catalytic activity test. The catalytic reaction was performed under atmospheric pressure in a fixed-bed reactor. Before the catalytic test, 1 g of the calcined catalyst was placed in the reactor and dried at 110 ˚C for 2 h in a flow of argon with a flow rate of 200 ml/min. Then, the catalyst was reduced at 400 ˚C for 2 h under pure hydrogen flow of 13 ml/min using a mass flow controller, and then cooled to ambient temperature. The activity of the catalysts was measured in the range of 30-350 ˚C under a feed stream of H_2:CO_2=4:1 with a gas hourly space velocity of 3,000 h^{-1}. Further, the methanation activity was determined at 350 ˚C for 1 h under the above

reaction conditions. The outflow gases were analyzed using a YL-GC6100 gas chromatograph equipped with a TCD detector and Porapack packed column.

3. Results and discussion

Catalyst characterizations

The textural properties of fresh Ni/Al, Ni/Al-15Y, and Ni-xCe/Al-15Y catalysts were summarized in Table 1. Actual catalyst composition determined by ICP-OES showed that Ni content was in a range of 8.94 - 13.4 wt% for all catalysts.

Table 1. Textural properties of the obtained Ni-xCe/Al-yY catalysts

Catalyst code	Nominal content, (wt%)				Experimental content* (wt%)	Crystalline size** (nm)
	Ni	Ce	Al	Y	Ni	NiO
Ni/Al	15.0	-	85.0	-	12.9	11.0
Ni/Al-15Y	15.0	-	70.0	15.0	13.4	5.80
Ni-1Ce/Al-Y	14.0	1.00	70.0	15.0	12.4	5.29
Ni-2Ce/Al-Y	13.0	2.00	70.0	15.0	11.9	4.36
Ni-5Ce/Al-Y	10.0	5.00	70.0	15.0	8.94	4.79

**Determined by ICP-OES analysis, ** Determined by XRD analysis*

Crystal structures of fresh Ni-xCe/Al-yY catalysts were characterized by XRD to identify the crystal phases. As shown in Figure 1, the diffractograms of Ni-xCe/Al-yY catalysts gave characteristic peaks corresponding to NiO, Al_2O_3, and Y_2O_3 phases but reflections due to CeO_2 crystallites were not found for the Ni-xCe/Al-yY catalysts. The Ce-promoted Ni-xCe/Al-yY catalysts improved nickel distribution, and reduced NiO crystalline size compared to Ni/Al catalyst. Furthermore, NiO crystal size of the Ni-2Ce/Al-15Y catalyst was the smallest of 4.36 nm. This result indicates that the Ce promoter increased the nickel distribution, and improved methanation activity with the Ni-2Ce/Al-yY catalysts.

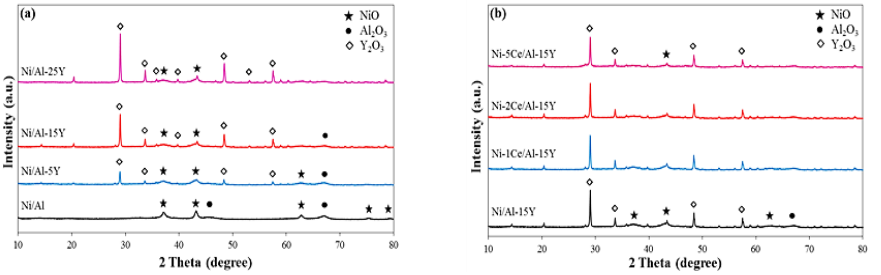

Figure 1. XRD patterns of the obtained fresh catalysts: (a) Ni/Al-yY and (b) Ni-xCe/Al-15Y

Spinel compounds formed by strong interactions between metal-support and support-support, such as nickel aluminate-$NiAl_2O_4$ and yttrium aluminate-$Y_3Al_5O_{12}$, were not observed by XRD analysis of all catalysts. These results suggested that the impregnation-co-precipitation method obstructed the strong interaction between nickel and support, and avoided from the formation of the inactive phases of nickel catalyst [3-4].

Catalytic performances

The catalytic activity results obtained with the Ni-xCe/Al-yY catalyst in CO_2 methanation are presented in Table 1. Reactions were performed at the temperature of 350 ˚C in the ambient pressure of H_2:CO_2 feed gas with the GHSV of 3000 h^{-1}. Ni/Al-yY catalysts reduced the methane formation temperature and increased methane productivity compared to Ni/Al catalysts without support additives. The addition of Y_2O_3 in the main support material improved the distribution of nickel catalyst (Figure 1), consequently increased the reaction activity of methanation. However, the most convenient content of the Y_2O_3 additive in Ni/Al-yY was 15%. Then, an effect of Ce promoter on Ni-xCe/Al-15Y was also investigated for CO_2 methanation.

Table 2. Comparison of catalytic activities of Ni-xCe/Al-yY catalysts at 350 ˚C

Catalysts	CO_2 conversion (%)	CH_4 yield (%)	CH_4 formation temperature (˚C)	Methane productivity (mmol/g_{cat})
Ni/Al	86.4	86.2	203	0.0692
Ni/Al-5Y	90.7	90.5	131	0.0812
Ni/Al-15Y	90.5	90.4	147	0.1013
Ni/Al-25Y	92.0	91.9	157	0.0919
Ni-1Ce/Al-15Y	91.1	90.5	155	0.1019
Ni-2Ce/Al-15Y	92.5	92.2	152	0.1041
Ni-5Ce/Al-15Y	86.4	86.3	140	0.0847

The catalytic activity of the prepared catalysts was dependent on the amount of support additives and catalyst promoter. As shown in Table 2, the Ni/Al-25Y and Ni-5Ce/Al-15Y catalysts with the highest contents of yttrium and cerium, had lower methane productivity compared to those of the Ni/Al-15Y catalyst. However, Ni-2Ce/Al-15Y gave the largest yield of CH_4 and its productivity at the present study condition. Figure 2 illustrates the effects of support addition and metal promoter on catalytic performance for CO_2 methanation.

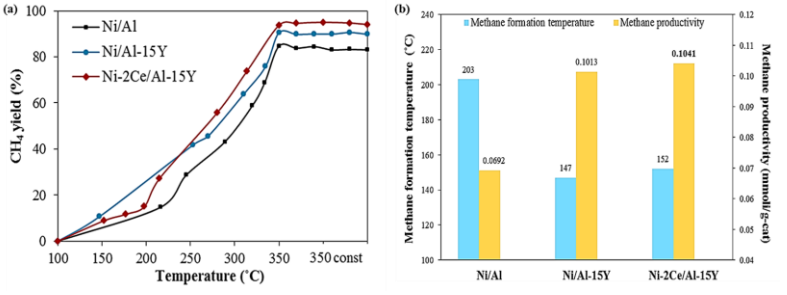

Figure 2. Effect of Ce promoter and Y support on methanation activity of Ni/Al catalyst: (a) CH_4 yield; (b) CH_4 productivity at 100-350 ˚C

The best performance of CO_2 methanation was achieved with the Ni-2Ce/Al-15Y catalyst and exhibited good stability compared to other catalysts in the 350 ˚C for 1 h. Compared to Ni/Al and Ni/Al-15Y catalysts, the cerium promoted - Ni-2Ce/Al-15Y catalyst increased CH_4 yield from 86.2% to 92.2% at 350 ˚C.

Conclusion

The Ni/Al_2O_3 and the cerium promoted nickel catalysts supported on mixed materials (Ni-xCe/Al-yY) were prepared by the method of impregnation-co-precipitation. The addition of Y_2O_3 in the main support material improved the distribution of nickel catalyst, consequently increased the reaction activity of methanation. However, the most convenient content of the Y_2O_3 additive in Ni/Al-yY was 15 wt%.

An effect of Ce promoter on Ni-xCe/Al-15Y was investigated for CO_2 methanation. The Ce promoter improved the catalytic performance of Ni/Al-15Y, in particular, when the nominal content of Ce was 2.0 wt%. The Ni-2Ce/Al-15Y catalyst gave the highest CO_2 conversion of 92.5% and the largest CH_4 yield of 92.2% at 350 ˚C.

References

[1] Zhou, L., Wang, Q., Ma, et al. CeO_2 Promoted Mesoporous Ni/γ-Al_2O_3 Catalyst and its Reaction Conditions For CO_2 Methanation. *Catalysis Letters* 2014; **145**(2):612-619.

[2] Liu, H., Zou, X., Wang, X., Lu, X., & Ding, W. Effect of CeO_2 addition on Ni/Al_2O_3 catalysts for methanation of carbon dioxide with hydrogen. *Journal of Natural Gas Chemistry* 2012; **21**(6):703-707.

[3] Buyan-Ulzii Battulga, Tungalagtamir Bold, Enkhsaruul Byambajav. Effect of Fe and Co promoters on CO methanation activity of nickel catalyst prepared by impregnation-co-precipitation method. *International Journal of Chemical Reaction Engineering* 2020; **18**(5-6):20200076.

[4] B.Buyan-ulzii, O.Daariimaa, Ch.Munkhdelger, G.Oyunbileg and B.Enkhsaruul. Effect of nickel precursor and catalyst activation temperature on methanation performance. *Mongolian Journal of Chemistry* 2018; **19**(45):12-18.

EXPERIMENTAL AND THEORETICAL ANALYSIS OF A REFRIGERATION SYSTEM WITH PHASE CHANGE MATERIAL (PCM) INTEGRATION

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Abstract
This study aims to improve the performance of a refrigeration system by increasing its compressor off time and, in that way, minimizing the electrical energy used by integrating the PCMs to the evaporator's exterior surface. The experiments were done in a test room using the laboratory scale refrigeration system to investigate the PCM charge and discharge rate and corresponding compressor on-off cycle duration. The test room air temperature was maintained at around 25°C by an air conditioner. The distilled water was chosen as PCM material. The theoretical results from the improved model were compared with experimental for the same operating conditions. Therefore, the advantages of integrating different quantity of PCM to the refrigeration system experimentally and theoretically were determined.
Key Words: *Energy-Saving; Performance Enhancement; Refrigeration System; Phase Change Material; Cold Cabin*

Introduction

Refrigeration, air-conditioning, and heat pump (RACHP) equipment and systems are widely used from small domestic equipment (e.g., refrigerators and room air-conditioners) to very large commercial and industrial systems (e.g., large building air-conditioning and food processing refrigeration). According to current estimates, RACHP equipment represents between 25% and 30% of the global consumption of electricity [1]. Regarding this energy consumption, energy-saving by thermal energy storage (TES) can be provided with the usage of phase change materials (PCM). The potential of the PCM to be used as a material for cold energy storage is investigated by the many researchers in literature [2,3].

Nomenclature	
A	area (m^2),
h	specific enthalpy (kJ/kg)
COP	coefficient of performance
$\dot{m}$	mass flow rate (kg/s)
n	rotation speed of the compressor (Hertz)
$\dot{Q}$	heat transfer rate (kW)
s	specific entropy (kJ/kg)
T	temperature (°C)
t_{off}	time interval of compressor's off-state for one compressor cycle (min)
t_{on}	time interval of compressor operation for one compressor cycle (min)
U	overall heat transfer coefficient ($W\ m^{-2}\ K^{-1}$)
V	compressor volume displacement (m^3)
$\dot{W}_c$	compressor power (W)
Greek Symbols	
η_C	isentropic efficiency of the compressor

η_V	volumetric efficiency
ρ	density (kg/m^3)
Subscripts	
1	inlet of the compressor
2	outlet of the compressor
3	outlet of the condenser
4	inlet of the evaporator
air	ambient air
cond.	condenser
ev	evaporator
is	isentropic
l	liquid
R	refrigerant
sc	sub-cooled
sh	superheat
tp	two-phase
v	vapour

2. Materials and Methods

2.1. Experimental study

The test rig was designed and installed to perform experiments on a cooling system, see Fig 1. The test rig consisted of an evaporator, compressor, condenser, low and high-pressure gauges, temperature gauges and indicators, flow meter, control panel parts. The inner volume of the cooling cabin is about 72 litres.

The thermostatic controller set point was adjusted so that the cabinet air temperature is maintained at 5°C. The experiments were performed in a closed room where the temperature is maintained almost constant about 25°C with an air conditioner.

Refrigerant mass flow rate, evaporator, compressor, and condenser temperatures were recorded by a data logging unit. Power consumption measured by the network analyzer device and the cabinet air temperature measured by the thermostatic controller were read from the LCD screens of the devices at the control panel.

Distilled water was chosen as PCM. Since the distilled water has a high latent heat of about 331 kJ/kg, it has remarkable potential for usage as a PCM [4]. In total, 1000 ml, PCM filled aluminium foil zip lock bags were placed on the evaporator to cover of evaporator tubes, as shown in Fig 1.

The purpose of using aluminium foil bags for the encapsulation was to improve heat transfer between evaporator surface-PCM and PCM-cabinet air. Besides being made of aluminium material, the flexible structure of PCM bags also increases the heat transfer by taking the form of the evaporator fins, thereby minimizing the possible air gaps. Before starting the experiments, PCMs were frozen horizontally.

Fig. 1. (a) view of the test rig; (b) placement of the PCM bags

2.2. Model of system components

The series of assumptions and equations used to model of the system are presented in Fig.2 . Components of the system such as compressor, evaporator, expansion valve and condenser are modelled separately by EES.

Compressor	Condenser	Expansion valve	Evaporator
Mass flow rate: $\dot{m}_R = \rho_R V_R \eta_V n$ Compressor power: $\dot{W}_c = \dot{m}_R(h_1 - h_2)$ Isentropic entropy of compressor outlet: $s_1 = s_{2,is}$ Isentropic compressor power: $\dot{W}_{c,s} = \dot{m}_R(h_1 - h_{2,is})$ Actual compressor work: $\dot{W}_c = \frac{W_{c,is}}{\eta_c}$ Assumptions: • Isentropic and volumetric efficiencies are kept constant. • The compression process is adiabatic.	The superheated region heat transfer: $\dot{Q}_{cond.,sh} = \dot{m}_R(h_2 - h_{2,v})$ The two-phase region heat transfer: $\dot{Q}_{cond.,tp} = \dot{m}_R(h_{2,l} - h_{2,v})$ Condenser outlet enthalpy, h_3 was computed by heat transfer in the subcooled region: $\dot{Q}_{cond.,sc} = \dot{m}_R(h_{2,l} - h_3) = U_{sc}A_{sc}(T_{2,l} - T_{air})$ Total heat transfer in the condenser: $\dot{Q}_{cond.} = \dot{Q}_{cond.,sh} + \dot{Q}_{cond.,tp} + \dot{Q}_{cond.,sc}$ Assumptions: • One-dimensional flow. • Heat transfer between refrigerant and pipes is neglected. • Pressure drop is neglected.	$h_3 = h_4$ Throttling process was considered in constant enthalpy and one dimensional.	Heat transfer on evaporator: $\dot{Q}_{ev} = \dot{m}_R(h_1 - h_4)$ Coefficient of performance: $COP = \frac{\dot{Q}_{ev}}{\dot{W}_c}$ Assumptions: • One dimensional flow. • Axial heat transfer between the evaporator tubes and the refrigerant is neglected.

Fig 2. model of the system

3. Results and Discussion

3.1. Effect of the PCM on the compressor on-off cycle

When the effect of the PCM on the cycles (on+off cycle) is compared, the time interval of one cycle (on+off cycle) was measured to be 23 minutes for with PCM case and 19 minutes for without PCM case. The compressor off time of one cycle is about 14 minutes for the system without PCM, while it is 18 minutes for the system with PCM, see Fig 3. This prolongation in the compressor off-time is a result of the absorption of the excess heat in the cabin by the PCM due to its phase change feature (solid to liquid) during compressor off-time. This prevents the cabin temperature from rising rapidly, so that extends the compressor off time; that is, PCM is utilized like an extra evaporator.

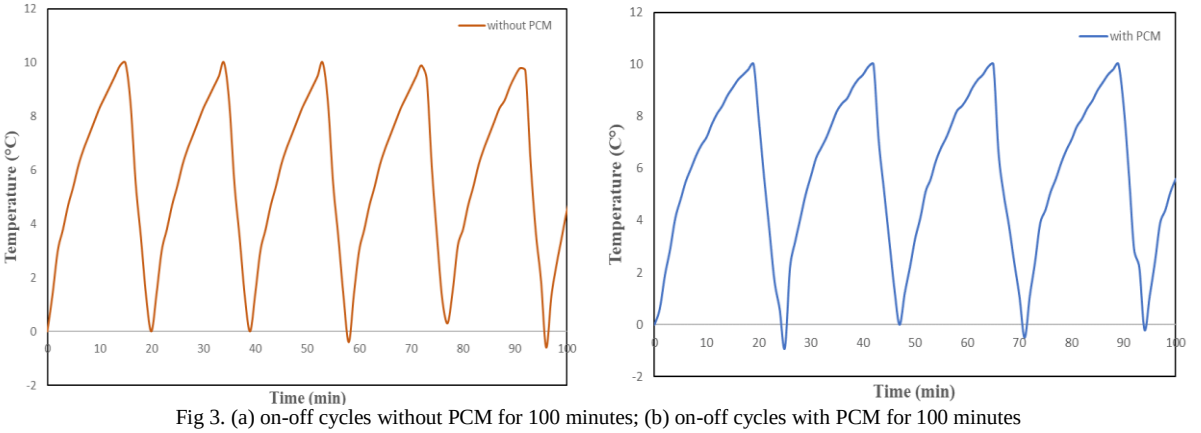

Fig 3. (a) on-off cycles without PCM for 100 minutes; (b) on-off cycles with PCM for 100 minutes

3.2. Energy consumption

Energy parameters for studied cases are summarized in Table 1. Experimental results were used to calculate the percentages of running time and daily energy saving by using equations below:

$$\text{Running time } (\%) = \frac{t_{on}}{t_{on}+t_{off}} x100, \qquad \text{Energy} - \text{saving } (\%) = \frac{\dot{W}_{PCM}-\dot{W}}{\dot{W}} x100$$

where $\dot{W}$ and $\dot{W}_{PCM}$ represent daily energy consumption without and with PCM, respectively. 16.7 % of energy saving was obtained by using PCM. Since the increase in compressor work is not excessive, the decrease in running time ratio compensates for this load on the system and provide energy saving.

Table 1. Energy parameters for without PCM and with PCM cases

Energy Parameters	Without PCM	With PCM
Compressor Power (W)	287 (from the model)	295 (from the model)
COP	3.1	2.7
Running Time (%)	26	22
The daily compressor on time (min)	379	313
The daily compressor off time (min)	1061	1127
Daily energy consumption (kWh/24 h)	1.8	1.5
Energy-saving (%)	-	16.7

4. Conclusions & Future Work

In this study, a test rig was designed and installed to perform the experiments of a refrigeration system with and without PCM. Also, a mathematical model of the test rig was proposed for both cases. Following conclusions have been obtained from this study:

- During the test period of 100 minutes, the number of cycles (on+off cycle) without PCM and with PCM was measured to be 5 and 4, respectively. The time intervals of the cycles (on+off cycle) were observed as 23 minutes for the PCM case and 19 minutes without the PCM case. The compressor off time of one cycle without PCM is about 14 minutes, while it is 18 minutes for PCM. Hence, the on-time of the compressor was found to be 5 minutes for both cases. Consequently, the running times of the system were calculated to be 22 % for the case with PCM and 26 % for the case without PCM.
- The prolongation in the off-time of the compressor was achieved, and this prolongation compensated the increase in the compressor work and also provided energy-saving. The energy savings were computed based on daily energy consumptions. For the case with PCM, energy-saving is calculated as 16.7 % compared to the case without PCM.
- In this study, obtained energy saving depends on the ambient temperature, the operating setting of the test rig, and the phase change temperature of PCM. All of these parameters should be considered for future studies. Also, the behaviour of the cabin air temperature with the integration of various quantity of PCM inside the cabin has to be observed and evaluated.

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References

[1] Briefing Note A The Importance of Energy Efficiency in the Refrigeration, Airconditioning and Heat Pump Sectors. United Nations Environment Programme May, 2018.

[2] Joybari, M., M., Haghighat, F., Moffat, J., Sra, P. (2015) Heat and cold storage using phase change materials in domestic refrigeration systems: The state-of-the-art review, Energy and Buildings, 106, 111-124.

[3] Ben-Abdallah, R., Leducq, D., Hoang, H.M., Fournaison, L., Pateau, O., Ballot-Miguet, B., Delahaye, A.,2019. Experimental investigation of the use of PCM in an open display cabinet for energy management purposes. Energy Conversion Management.198, 111909.

[4] Yusufoglu, Y., Apaydin, T., Yilmaz, S., Paksoy, H. O.,2015. Improving performance of household refrigerators by incorporating phase change materials. International Journal of Refrigeration, 57, 173-185.