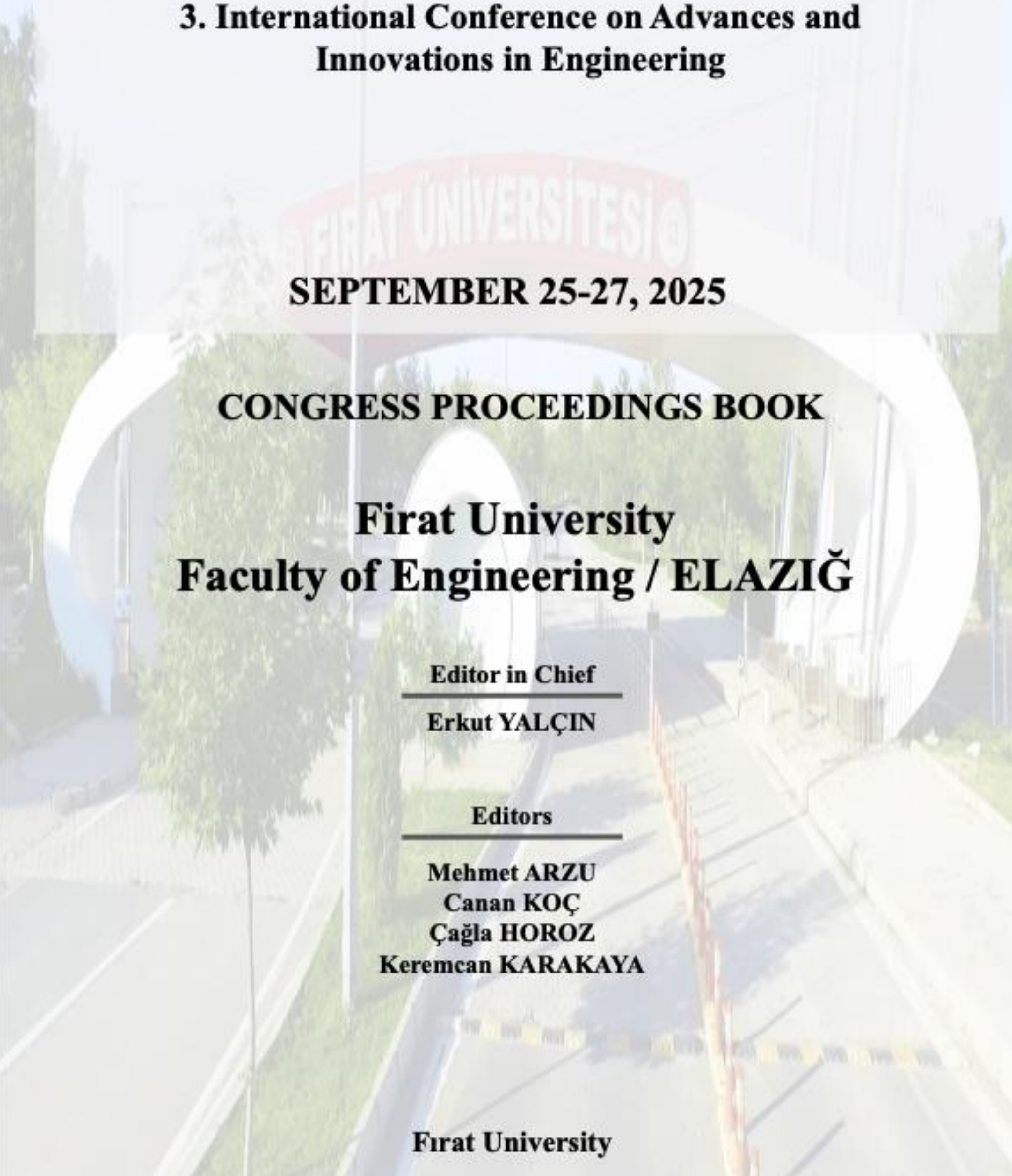
3. ICAIE

3. International Conference on Advances and Innovations in Engineering



FIRAT ÜNİVERSİTESİ

SEPTEMBER 25-27, 2025

CONGRESS PROCEEDINGS BOOK

Firat University
Faculty of Engineering / ELAZIĞ

Editor in Chief

Erkut YALÇIN

Editors

Mehmet ARZU
Canan KOÇ
Çağla HOROZ
Keremcan KARAKAYA

Fırat University

International Conference on Advances and Innovations in Engineering

3.ICAIE

Conference Date 25-27 September 2025

15 June 2025
Deadline for abstract submission

30 June 2025
Deadline for full-text submission

www.icaie.org.tr **2025**

Place: Fırat University, Atatürk Culture and congress Center

INTRODUCTION

Dear Distinguished Delegate,

The third edition of the International Conference on Advances and Innovations in Engineering (ICAIE) was held between 25-27 September 2025 at Fırat University Faculty of Engineering, Elazığ.

International Conference on Advances and Innovations in Engineering is an international scientific forum of distinguished scholars engaged in scientific, engineering and technological research, dedicated to the furtherance of science, engineering and technology. The academic research conference since its inception is at the cutting edge of international nonprofit scientific, engineering and technological progress to promoting excellence in science.

The conference plays an influential role in science and promotes developments in science, engineering and technology in a wide range of ways. The conference aims to foster research in the area of science and technology and its impact to mainstream human activities. Specifically, it serves as a venue for discussions and exchange of ideas in current issues in science and technology.

All full paper and abstract submissions to the conference are peer reviewed and refereed and evaluated based on originality, research content and correctness, relevance to contributions, and readability. In this content the full paper and abstract submissions are chosen based on technical merit, interest, applicability and how well they fit a coherent and balanced technical program. The accepted papers after rigorous peer reviewing process have been published in the refereed international conference proceedings

Chair of ICAIE Committee
Prof. Dr. Ebru AKPINAR

Honour Committee

Prof. Dr. Fahrettin GÖKTAŞ, Rector
Prof. Dr. Mehmet YILMAZ, Vice Rector

Committee Members of the ICAIE

Chair of Conference

Prof. Dr. Ebru AKPINAR, Dean

Organizing Committee

Abayhan BURAN, Fırat University (Bioengineering)
Ahmet ÇINAR, Fırat University (Computer Engineering)
Akın ODABAŞI, Fırat University (Metallurgical and Materials Engineering)
Arif GÜLTEN, Fırat University (Electrical and Electronics Engineering)
Arkadiusz DOBRZYCKI, Poznan University
Ayla ÖZER, Mersin University (Chemical Engineering)
Ayşe Nur BAKIRCI
Ayşe Vildan BEŞE, Atatürk University (Chemical Engineering)
A. Garci HERNANDEZ, RWTH Aachen University
Baha Vural KÖK, Fırat University (Civil Engineering)
Buğrahan Fatih FURTANA, Fırat University (Civil Engineering)
Buket ERZEN, Fırat University (Chemical Engineering)
Burçak EBİN, Chalmers University
Bünyamin ERGEZİN, Fırat University (Mechatronics Engineering)
Canan KOÇ, Fırat University (Software Engineering)
Celal KISTAK, Fırat University (Mechanical Engineering)
Cenk YANEN, Fırat University (Mechanical Engineering)
Cevdet AKOSMAN, Fırat University (Chemical Engineering)
Çağla HOROZ, Fırat University (Software Engineering)
Çağrı KAYMAK, Fırat University (Mechatronics Engineering)
Deniz ÜNER, Middle East Technical University (Chemical Engineering)
Dursun ÖZER, Fırat University (Chemical Engineering)
Emrah ÇELİK, Fırat University (Metallurgical and Materials Engineering)
Emre GÜÇLÜ, Fırat University (Computer Engineering)
Ercan AYDOĞMUŞ, Fırat University (Chemical Engineering)
Erkin EREN, Fırat University (Civil Engineering)
Erkut YALÇIN, Fırat University (Civil Engineering)
Fatih DEMİR, Fırat University (Software Engineering)
Fatih KAYA, Fırat University (Chemical Engineering)
Fatih ÖZYURT, Fırat University (Software Engineering)
Fethi KAMIŞLI, Fırat University (Chemical Engineering)
Filiz KAR, Fırat University (Chemical Engineering)
Fulvio PARISI, Naples Federico II Via Claudio University
Gamze SAK, Fırat University (Chemical Engineering)
Gamze UYGUR
Gizem Gül KATIRCIOĞLU, Fırat University (Mechanical Engineering)
Gülbeyi DURSUN, Fırat University (Chemical Engineering)
Güngör YILDIRIM, Fırat University (Computer Engineering)
Hamdi Soner ALTUNDOĞAN, Fırat University (Bioengineering)

Hasan YETİŞ, Fırat University (Computer Engineering)
Hossein MOAYEDI, Duy Tan University
Hüseyin KARACA, İnönü University (Chemical Engineering)
İlhan AYDIN, Fırat University (Computer Engineering)
İnanç ÖZGEN, Fırat University (Bioengineering)
İnci Türk TOĞRUL, Batman University (Petroleum and Natural Gas Engineering)
Keremcan KARAKAYA, Fırat University (Artificial Intelligence and Data Engineering)
Kıvanç DOĞAN, Fırat University (Electrical and Electronics Engineering)
Kübra BULUT, Fırat University (Civil Engineering)
Kübra ŞİŞLİOĞLU, Fırat University (Food Engineering)
Loke Kok FOONG, Duy Tan University
Mahmut KAYA, Fırat University (Artificial Intelligence and Data Engineering)
Mansour MOSALLANEZHAD, Shiraz University
Mehmet Ali ERTÜRK, Fırat University (Geological Engineering)
Mehmet ARZU, Fırat University (Artificial Intelligence and Data Engineering)
Mehmet Deniz TURAN, Fırat University (Metallurgical and Materials Engineering)
Mehmet ERDEM, Hacettepe University (Environmental Engineering)
Mehmet KALENDER, Fırat University (Bioengineering)
Mehmet KARAKÖSE, Fırat University (Computer Engineering)
Mehmet KÖKÜM, Fırat University (Geological Engineering)
Mehtap TANYOL, Munzur University (Environmental Engineering)
Melek YILGIN, Fırat University (Chemical Engineering)
Mert İNCİDELEN, Fırat University (Artificial Intelligence and Data Engineering)
Merve YILDIRIM, Fırat University (Electrical and Electronics Engineering)
Mesut GÖR, Fırat University (Civil Engineering)
Mete Onur KAMAN, Fırat University (Mechanical Engineering)
Mohammed Abdullahi Mu'azu, Hafr Al-Batin University
Muhammed KARATON, Fırat University (Civil Engineering)
Muhammad Masood RAFI, NED ve Teknoloji University
Mukaddes KARATAŞ, Fırat University (Chemical Engineering)
Musharraf ZAMAN, Oklahoma University
Mustafa YEGİN, Fırat University (Environmental Engineering)
M. Barbaros DURMUŞ, Firat University (Environmental Engineering)
M. Sefa ÇETİN, Fırat University (Electrical and Electronics Engineering)
Neslihan DURANAY, Fırat University (Chemical Engineering)
Nevin ÇELİK, Fırat University (Mechanical Engineering)
Nicola TARQUE, Pontifical Catholic University
Niyazi Furkan BAR, Fırat University (Computer Engineering)
Nuno MENDES, Minho University
Nurhan ARSLAN, Fırat University (Chemical Engineering)
Özge HANAY, Fırat University (Environmental Engineering)
Pranshoo SOLANKI, Illinois State University
Ragip İNCE, Fırat University (Civil Engineering)
Ramazan ORHAN, Fırat University (Chemical Engineering)
Rouzbeh GHABCHI, South Dakota State University
Seda ARSLAN TUNCER, Fırat University (Software Engineering)
Sibel ASLAN, Fırat University (Environmental Engineering)
Soheil GHAREH, Payame Noor University
Şeyda TAŞAR, Fırat University (Chemical Engineering)
Zeynep KARACA, Fırat University (Computer Engineering)

Scientific Committee

A. Didem KILIÇ, Fırat University
A. Erçin ERSUNDU, Yıldız Technical University
A. Sükran DEMIRKIRAN, Sakarya University
Abdullah Hilmi LAV, İstanbul Technical University
Abdullah SAR, Fırat University
Abdülhakim ZEYBEK, Muş Alparslan University
Abdulkadir SENGUR, Fırat University
Abuzer ÇALIŞKAN, Fırat University
Adem ATMACA, Gaziantep University
Ahmet Arif AYDIN, İnönü University
Ahmet Bedri ÖZER, Fırat University
Ahmet Burak TATAR, Fırat University
Ahmet Can ALTUNIŞIK, Karadeniz Technical University
Ahmet ÇINAR, Fırat University
Ahmet HASÇALIK, Fırat University
Ahmet Koca, Fırat University
Ahmet ORHAN, Fırat University
Ahmet ŞAŞMAZ, Fırat University
Ahmet TÜRK, Manisa Celal Bayar University
Ahmet Top, Fırat University
Ahmet YILDIZ, Fırat University
Akın Odabaşı, Fırat University
Ali ARI, İnönü University
Ali TOPAL, Dokuz Eylül University
Ali Kaya GÜR, Fırat University
Alp Buğra Aydın, Fırat University
Alper K. TANYILDIZI, Fırat University
Arif GÜLTEN, Fırat University
Arzu Fırat ERSOY, Karadeniz Technical University
Arzu Yadigar DURSUN, Fırat University
Aslı GİRAY, Alanya Alaaddin Keykubat University
Atike NAZİK, Çukurova University
Ayberk KAYA, Recep Tayyip Erdoğan University
AYÇA AK, Marmara University
Aydın ÇITLAK, Fırat University
Aydın DİKİCİ, Fırat University
Ayhan AKBAL, Fırat University
Ayhan ORHAN, Fırat University
Aykut ÖZPOLAT, Fırat University
Aynur UÇAR, Fırat University
Ayşe Ruşen DURUCAN, Fırat University
Ayşe BİÇER, Malatya Turgut Özal University
Ayşegül UÇAR, Fırat University
Aytekin ÇELİK, Fırat University
Aziz AKSOY, Malatya Turgut Özal University
Aziz SARAÇOĞLU, Fırat University
Baha Vural KÖK, Fırat University
Bahar DEMİREL, Fırat University
Bahadır YILMAZ, Bursa Technical University
Bahtiyar ÖZTÜRK, Ondokuz Mayıs University
Banu TAŞKAN, Fırat University

Barış KARAKAYA, Fırat University
Betül ÇİÇEK ÖZKAN, Fırat University
Belkiz TORĞUL, Erzurum Technical University
Beyda TAŞAR, Fırat University
Bihter DAŞ, Fırat University
Bilal ALATAŞ, Fırat University
Bircan ÇALIŞIR, Fırat University
Burak KIYAK, Fırat University
Burak ŞENGÖZ, Dokuz Eylül University
Burhan ERGEN, Fırat University
Bünyamin AKGÜL, Fırat University
C. Fahir ARISOY, İstanbul Technical University
Cafer BAL, Fırat University
Calibe KOÇ TAŞGIN, Fırat University
Canan DÜLGER, Izmir University of Economics
Cebeli ÖZEK, Fırat University
Cemal BÖLÜCEK, Balıkesir University
Cengizhan DURUCAN, Fırat University
Cengiz YILDIZ, Fırat University
Cenk YANEN, Fırat University
Cevdet Emin EKİNCİ, Fırat University
Cihangir KALE, Fırat University
Cihan ÖZEL, Fırat University
Çetin GENÇER, Fırat University
Çetin ÖZAY, Fırat University
Davut HANBAİ, İnönü University
Dicle Bal AKKOCA, Fırat University
Duygu KAYA, Fırat University
Ebubekir ERDEM, Fırat University
EMİNE CENGİL, Bitlis Eren University
Emine Işıl TOPAL, Fırat University
Emre TURGUT, Fırat University
Ender SUVACI, Eskisehir Technical University
Engin AVCI, Fırat University
Engin GÜRTEKİN, Fırat University
Engin Ünal, Fırat University
Enis GÜNAY, Erciyes University
Ercan AKSOY, Fırat University
Erdal ÖBEK, Fırat University
Erdal ÖZBAY, Fırat University
Erdinç ARICI, Fırat University
Ergin TAŞKAN, Fırat University
Erhan AKIN, Fırat University
Erkan AKBAL, Fırat University
Erkan DENİZ, Fırat University
Erkan DUMAN, Fırat University
Erkan TANYILDIZI, Fırat University
Erkut SAYIN, Fırat University
Erman ÇELİK, Fırat University
Ertan BÜTÜN, Fırat University
Eser SERT, Malatya Turgut Özal University
Esra Tuğrul TUNÇ, Fırat University
Esra YILDIRIM, Fırat University

Fahri ÖZKAN, Fırat University
Faruk KARACA, Fırat University
Fatih ERTAM, Fırat University
Fatih ÖZKAYNAK, Fırat University
Ferhat UÇAR, Fırat University
Ferkan SİPAHİ, Gümüşhane University
Feyza ALTUNBEY ÖZBAY, Fırat University
Filiz ÖZGEN, Fırat University
Figen BALO, Fırat University
Furkan SARSILMAZ, Fırat University
Galip AYDIN, Fırat University
Gonca ÖZMEN KOCA, Fırat University
Gökay BAYRAK, Bursa Technical University
Gökhan BAŞMAN, ETİ Krom
Gökmen TAYFUR, Izmir Institute of Technology
Gül TOSUN, Fırat University
Güllü BOZTAŞ, Fırat University
Gülşad Uslu ŞENEL, Fırat University
Gülşah ÇAKMAK, Fırat University
Gülşah KARADUMAN, Fırat University
Gültekin GÖLLER, İstanbul Technical University
H. Lütfi YÜCEL, Fırat University
H. Suha AKSOY, Fırat University
H.Soner ALTUNDOĞAN, Fırat University
Hakan ÇELİK, Fırat University
Murat KARACASU, Eskişehir Osmangazi University
Halil İbrahim YAMAÇ, Fırat University
Hanbey HAZAR, Fırat University
Hanifi GÜLDEMİR, Fırat University
Hanzade AÇMA, İstanbul Technical University
Harun TANYILDIZ, Fırat University
Hasan ÇELİK, Fırat University
Hasan GÜLER, Fırat University
Hasan YETİŞ, Fırat University
Haşim PİHTİLİ, Fırat University
Haydar EREN, Fırat University
Hayrettin CAN, Fırat University
Hediye AYDIN, Kütahya Dumlupınar University
Hikmet ESEN, Fırat University
Hülya BİÇER, Kütahya Dumlupınar University
Hümeyra ŞAHİN, Fırat University
Hüseyin ALTUN, Fırat University
Hüseyin ÇİMENOĞLU, İstanbul Technical University
Hüseyin SEVİNÇ, Fırat University
Hüseyin YAĞLI, Gaziantep University
İbrahim BERKAN AYDİLEK, Harran University
İbrahim TÜRKMEN, Balıkesir University
İbrahim TÜRKOĞLU, Fırat University
İhsan DAĞTEKİN, Fırat University
İlhan AYDIN, Fırat University
İlhan Fırat KILINÇER, Fırat University
Kazım TÜRK, İnönü University
Kürşat Esat ALYAMAÇ, Fırat University

Latif ÖZLER, Fırat University
Levent TAŞÇI, Fırat University
Leyla KALENDER, Fırat University
M. Cihat TUNA, Fırat University
Bay Deniz TURAN, Fırat University
M. Emin EMİROĞLU, Fırat University
M. Erbil ÖZCAN, Fırat University
M. Salih KESKİN, Dicle University
Mahmut Temel ÖZDEMİR, Fırat University
Mediha İPEK, Sakarya University
Mehmet ALTUNBEY, Fırat University
Mehmet ARSLAN, Karadeniz Technical University
Mehmet CEBECİ, Fırat University
Mehmet ÇAVAŞ, Fırat University
Mehmet DAŞ, Fırat University
Mehmet ESEN, Fırat University
Mehmet EROĞLU, Fırat University
Mehmet GEDİKPINAR, Fırat University
Mehmet H. KORKUT, Fırat University
Mehmet KAYA, Fırat University
Mehmet POLAT, Fırat University
Mehmet Sait SÖYLEMEZ, Gaziantep University
Mehmet Sinan BİLGİLİ, Yıldız Technical University
Mehtap MURATOĞLU, Fırat University
Melahat BEYARSLAN, Fırat University
Melek URAL, Fırat University
Meral ÖZEL, Fırat University
Mert GÜRTÜRK, Fırat University
Mete KALYONCU, Konya Technical University
Mete Onur KAMAN, Fırat University
Metin GÜRÜ, Gazi University
Miray Çelikbilek ERSÜNDÜ, Yıldız Technical University
Muammer GÖKBULUT, Fırat University
Muammer TÜRKOĞLU, Samsun University
Muhammed ATAR, Fırat University
Muhammet BAYKARA, Fırat University
Muhammed Emre ÇOLAK, Fırat University
Muhammed Fatih TALU, İnönü University
Muhammed Furkan KÜÇÜK, Fırat University
Muhammed TALO, Fırat University
Muhammed ULUCAN, Fırat University
Muhammed YILDIRIM, Malatya Turgut Özal University
Muhammet AYDIN, Fırat University
Muhammet KARATON, Fırat University
Muharrem AKGÜL, Balıkesir University
Muhsin Tunay GENÇOĞLU, Fırat University
Murat AYDOĞAN, Fırat University
Murat BAYDOĞAN, İstanbul Technical University
Murat ELİBOL, Ege University
Murat KARABATAK, Fırat University
Murat KARACASU, Eskisehir Osmangazi University
Murat ŞEN, Fırat University
Murat Yavuz SOLMAZ, Fırat University

Musa ÇIBUK, Bitlis Eren University
Musa YETKİN, Fırat University
Mustafa AY, Fırat University
Mustafa BOYRAZLI, Fırat University
Mustafa Can BİNGÖL, Burdur Mehmet Akif Ersoy University
Mustafa GÜR, Fırat University
Mustafa İNALLI, Fırat University
Mustafa KANIK, Fırat University
Mustafa KAYA, Fırat University
Mustafa KAPTANOĞLU, Fırat University
Mustafa Selman AYDOĞAN Balıkesir University
Mustafa TUNCER, Kütahya Dumlupınar University
Mustafa TUNÇ, Fırat University
Mustafa TÜRK, Fırat University
Mustafa ULAŞ, Fırat University
Müge Elif FIRAT, Fırat University
Müjdat FIRAT, Fırat University
Müslüm ARKAN, İnönü University
Müslün Sara TUNÇ, Fırat University
Namık AYSAL, İstanbul University
Necip ÜNLÜ, İstanbul Technical University
Nevin ÇELİK, Fırat University
Nida KATI, Fırat University
Nihat KAYA, Fırat University
Nihat TOSUN, Fırat University
Nilüfer KOÇER, Fırat University
Niyazi ÖZDEMİR, Fırat University
Oğuz YAKUT, Fırat University
Oğuzhan HASANÇEBİ, Middle East Technical University
Oğuzhan KELEŞTEMUR, Fırat University
Oktay YİĞİT, Fırat University
Onuralp YÜCEL, İstanbul Technical University
Orhan ATİLA, Fırat University
Orhan ÇAKAR, Fırat University
Orhan YAMAN, Fırat University
Osman YİĞİD, Bitlis Eren University
Ö. Faruk DURSUN, İnönü University
Ömer GÜLER, Munzur University
Ömer KELEŞOĞLU, Fırat University
Ömer Sinan ŞAHİN, Konya Technical University
Ömer ŞAHİN, İstanbul Technical University
Ömer Yavuz BOZKURT, Gaziantep University
Ömür AYDOĞMUŞ, Fırat University
Özal YILDIRIM, Fırat University
Özge Erdoğan YAMAÇ, Fırat University
Özge HANAY, Fırat University
Özgür AVŞAR, Eskisehir Technical University
Özgür KARADUMAN, Fırat University
Özgür YILDIZ, Yıldız Technical University
Özkan ÖZDEMİR, Sakarya University of Applied Sciences
Özlem Öztekin OKAN, Fırat University
Özlem TEPE, Fırat University
Pakistanlı TURGUT, İnönü University

Ragıp İNCE, Fırat University
Recep ARTIR, Marmara University
Remzi TÜNTAŞ, Van Yüzüncü Yıl University
Resul ÇÖTELİ, Fırat University
Resul DAŞ, Fırat University
Reşat ÇELİKEL, Fırat University
Sadettin KAPUCU, Gaziantep University
Sencer ÜNAL, Fırat University
Serdar Ethem HAMAMCI, İnönü University
Serkan ERDEM, Fırat University
Servet TUNCER, Fırat University
Servet YILDIZ, Fırat University
Sevcan KÜRÜM, Fırat University
Sibel ASLAN, Fırat University
Sibel KAYGILI, Fırat University
Sinem AKYOL, Fırat University
Soner BUYTOZ, Fırat University
Şaban TANYILDIZI, Fırat University
Şengül DOĞAN, Fırat University
Taha TAŞKIRAN, Ankara Yıldırım Beyazıt University
Tahsin BOYRAZ, Sivas Cumhuriyet University
Taner ALATAŞ, Fırat University
Taner TUNCER, Fırat University
Tuba DEMİR, Fırat University
Turan GÜRGENÇ, Fırat University
Turgay KAYA, Fırat University
Tülay YILDIRIM, Yıldız Technical University
Tülay YILDIZ, Fırat University
Türker TUNCER, Fırat University
Said ERAY, Sivas University of Science and Technology
Seda ARSLAN TUNCER, Fırat University
Sedat SAVAŞ, Fırat University
Selçuk ALEMDAĞ, Gümüşhane University
Selçuk KARATAŞ, Fırat University
U. Teoman AKSOY, Fırat University
Uğur ÇALIGÜLÜ, Fırat University
Utku KÖSE, Süleyman Demirel University
V.Cem BAYDOĞAN, Fırat University
Vedat ÇELİK, Fırat University
Vedat SAVAŞ, Fırat University
Venhar ÇELİK, Fırat University
Veyis SELEN, Fırat University
Yakup DEMİR, Fırat University
Yaman AKBULUT, Fırat University
Yasemin TOPÇUOĞLU, Fırat University
Yasin VAROL, Fırat University
Yaşar NUHOĞLU, Yıldız Technical University
Yavuz EROL, Fırat University
Yılmaz YILDIRIM, Zonguldak Bülent Ecevit University
Yunus Emre BENKLİ, Atatürk University
Yunus ERKUŞ, Fırat University
Yusuf CALAYIR, Yalova University
Yüksel ESEN, Fırat University

Z. Fuat TOPRAK, Dicle University
Zeynep Bala DURANAY, Fırat University
Zülfü GÜROCAK, Fırat University
Zümriye AKSU, Hacettepe University

Session Chairmans

Hamdi Soner ALTUNDOĞAN

Gülbeyi DURSUN

Fatih DEMİR

Filiz KAR

Ragip İNCE

Melek YILGIN

Nevin ÇELİK

Arif GÜLTEN

İnanç ÖZGEN

Muhammet KARATON

İlhan AYDIN

Mehmet Deniz TURAN

Erkut YALÇIN

Mete Onur KAMAN

Özge HANAY

Baha Vural KÖK

Seda ARSLAN TUNCER

Cevdet AKOSMAN

CONTENTS

Production and Characterization of Chitosan-TiO_2 Composite Beads 15

Water Sustainability 16

Risk Assessment in Limestone Quarries Using Fine–Kinney Method: Occupational Health and Environmental Considerations 17

Investigation of Experimental and Theoretical Spectral Data of 2-Tridecyl-4,5-Dihydro-1H-Imidazole 18

In Silico Molecular Docking of 2-Tridecyl-4,5-Dihydro-1H-Imidazole For Possible Treatment of Alzheimer's Disease 21

Investigation of the Potential Activity of 3-((1H-benzotriazol-1-yl)methyl-4-ethyl-1H-1,2,4-triazol-5(4H)-thione Against MCF-7 and L1210 Cancer Cells 24

Behavior of Sodium Bentonite in Acidic and Alkaline Environments: Modeling Filtrate Properties with Machine Learning 26

Modeling of Biochar Production Process Efficiency from Tea Pulp and Almond Outer Shell Using Machine Learning Methods 27

The Role of Activated Carbon in Supercapacitor Technology 29

Thermal Convection Zone Detection for Glider Soaring Control via Seven-Class Cloud Type Classification Using Swin Transformer on Ground-Based Images 30

FireStageNet: A Transformer-Based Deep Learning Approach for Image-Based Fire Stage Classification 32

Photocatalysis Applications of MnOx-Decorated Biphasic Nanostructures: Methylene Blue Model 33

Removal of Dyestuff from Aqueous Solutions using Magnetic Cerium Particles 35

Chemical Characterization of Lignocellulosic Biomass for Sustainable Biofuel Production 37

Green Synthesis of Silver Nanoparticles from Walnut Shell Extract and Their Comparative Performance in PLA/Epoxy and PLA/PEG Biocomposites 39

Faunistic Contribution to Turkish Cicadellidae: First Record of Frutioidia (Frutioidia) bisignata (Mulsant & Rey, 1855) in Bingöl 41

Synthesis of 1-(4-methoxybenzoyl)-4-(naphthalen-1-yl) thiosemicarbazide Compound and Investigation of its Experimental and Theoretical Spectra 44

Thermochemical Valorization of Microalgal Biomass: Insights into Torrefaction and Pyrolysis Pathways for Sustainable Bioenergy Production (Mini- Review) 47

Fabric Defect Detection Using Synthetic Defect Augmentation and Deep Learning 49

Production and Characterization of Chitosan-TiO_2 Composite Beads

Nuri BOZKURT[1], Gamze SAK[2], Şeyda TAŞAR[3], Gülbeyi DURSUN[5]

[1,2,3,4] Chemical Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[1]sur59.tra61@gmail.com, [2]gsak@firat.edu.tr, [3]sydtasar@firat.edu.tr, [4]gdursun@firat.edu.tr
[1](ORCID: 0000-0000-0000-0000), [2](ORCID: 0009-0008-4812-0091), [3](ORCID: 0000-0003-3184-1542), [4](ORCID: 0000-0001-7788-9766)

Abstract

The increase in industrialization and various factories and industrial centers has led to the pollution of water resources including seas, oceans, groundwater, and lakes, which threaten the life of living organisms. Azo dyes, which are widely used in the textile industry, have a significant negative impact on water resources and the environment. Azo dyes, produced by combining the diazonium compound with an aromatic amine or phenol, are important synthetic organic colorants widely used in various applications such as cosmetics, gasoline, leather, foodstuffs, textiles, paper, and additives. However, textile wastes containing azo dyes create an undesirable situation due to their colors and the possibility of reduction to carcinogenic aromatic amines. Therefore, the pollution of water resources increases environmental pollution and this situation increases the interest in various wastewater treatment techniques including oxidation and biological processes, coagulation/flocculation, adsorption, electrochemical degradation, and photocatalytic mineralization. However, traditional methods such as coagulation/flocculation and adsorption only allow the phase transformation from liquid to solid without mineralizing the dye. In addition, biological processes take a long time and require high energy, so electrochemical oxidation is expensive. Photocatalytic degradation of textile dyes is a wastewater treatment technique widely used by developed countries and is considered an environmental solution in the literature. The photocatalytic degradation technique is widely preferred due to manageable process conditions, low cost, and environmental sustainability. In particular, the use of UV-C light is one of the most effective methods to degrade dyes and other soluble organic pollutants from water resources and wastewater. Studies on photocatalytic materials generally focus on the high photocatalytic activity and chemical durability of semiconductor catalysts. However, the potential advantages of creating hybrid structures with biopolymer-based materials are being investigated to increase the efficiency and regeneration efficiency of semiconductor catalysts. Chitosan attracts attention as a matrix material in photocatalytic applications due to its biodegradability, non-toxicity, and environmentally friendly properties. In previous studies, it was observed that the structural and optical properties of chitosan-semiconductor photocatalyst composites were improved, but studies on the kinetic and thermodynamic behavior of these materials in dye degradation were limited. In addition, it was determined in the literature that a systematic comparison between beads in the production processes of chitosan-based photocatalysts was lacking.

In this study, it was aimed to create an innovative, sustainable, and highly efficient photocatalyst by combining chitosan, an environmentally friendly and biodegradable biopolymer, with TiO_2, which has a strong oxidation capacity. In this context, the structural and morphological properties of the beads produced under different conditions (crosslinker ratio, deacetylation degree, etc.) were tried to be characterized. The surface structure, chemical composition, and thermal stability of the beads were examined in detail using methods such as Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and Thermogravimetric Analysis (TGA). In photocatalytic performance tests, the degradation efficiency of a commonly used azo dye such as reactive black 5 (RB5) under UV light was comparatively evaluated for each bead. Degradation efficiency was monitored with UV-Vis spectroscopy and TOC over time. The findings revealed that titanium dioxide-doped chitosan beads can be effectively used as photocatalysts in the photocatalytic degradation process for wastewater treatment, reduction of environmental pollution, and sustainable water management.

Keywords: chitosan, photocatalytic degradation, TiO_2, reactive black 5 (RB5), TOC, FTIR

---

[1] Corresponding author

Water Sustainability

Umay HALİSDEMİR [1], Fatih KAYA[2]

[1] Environmental Engineering Department, Engineering Faculty, Atatürk University, Erzurum, TURKEY.
[2] Chemical Engineering Department, Engineering Faculty, Fırat University, Elazığ, TURKEY.
[1]umayhalisdemir@gmail.com, [2]fatihkaya@firat.edu.tr
[1](ORCID: 0000-0002-0673-6233), [2](ORCID: 0000-0002-4063-8362)

Abstract

The accelerating pace of industrialization and global population growth continues to drive an increasing demand for water. In contrast, the limited availability of freshwater resources, coupled with environmental stressors such as global warming and recurring regional droughts, presents critical threats to the sustainability of water. This situation has steadily elevated the strategic significance of water resources worldwide. The concept of sustainability encompasses the efficient, balanced, and responsible use of all resources involved in production and consumption processes—within the boundaries of environmental limits, while promoting economic development and prioritizing social equity. It also entails the post-use recovery and recycling of these resources to ensure their preservation for future generations. Within this framework, water sustainability refers to the long-term, balanced, and integrated management of existing water resources in a way that meets societal needs and supports economic development—without compromising the ecological integrity of natural systems. This approach involves preserving water quality and quantity, ensuring efficient and effective use, recycling treated wastewater, and supporting the water cycle in harmony with natural processes. The aforementioned global importance of water is also underscored by alarming projections. According to the United Nations' World Water Development Report 2025, up to three billion people could be directly affected by water scarcity by 2030. Additionally, the Global Commission on the Economics of Water estimates that global water demand may exceed supply by 40% by 2030. These figures reveal that water is not only vital in terms of the supply-demand balance, but also a crucial factor for economic and social sustainability. In the case of Türkiye, the annual per capita water availability is approximately 1,200 m³, placing the country in the category of water-stressed nations. Climate change, irregular precipitation patterns, and inefficient water use have led to severe challenges, particularly in agricultural production and potable water supply. The Ministry of Agriculture and Forestry has reported a drop of over 30 meters in groundwater levels in several areas of Central and Southeastern Anatolia. In response, Türkiye launched a National Water Efficiency Mobilization Campaign in 2023, targeting reductions in water losses from drinking water networks and promoting modern irrigation systems. However, TÜBİTAK-supported research indicates that for such technical measures to produce sustainable outcomes, they must be accompanied by participatory governance, data-driven planning, and behavioral transformation. In conclusion, water sustainability on a global scale is not merely a biological necessity—it is a multi-dimensional strategic issue essential for peace, economic growth, and resilient societies. In Türkiye's context, water sustainability must now go beyond environmental policy and be embedded at the core of development strategies. To both adapt to climate risks and secure long-term social and economic stability, the integrated, equitable, and effective management of water is of paramount importance. Alongside national policies, regional cooperation and science-based solutions will be key to strengthening Türkiye's water security.

Keywords: water, sustainability, water strategy

---

[1] Corresponding author

Risk Assessment in Limestone Quarries Using Fine–Kinney Method: Occupational Health and Environmental Considerations

Vedat KARAHAN[1], Ercan AYDOĞMUŞ[2]

[1,2]Department of Chemical Engineering, Faculty of Engineering, Fırat University, 23119, Elazığ, Türkiye.
[1]vdtkrhn@gmail.com, [2]ercanaydogmus@firat.edu.tr
[1](ORCID: 0000-0002-0913-7826), [2](ORCID: 0000-0002-1643-2487)

Abstract

This study focuses on the assessment and evaluation of occupational health and safety risks in limestone quarries through the application of the Fine–Kinney Method. Within the scope of the research, risk analyses were conducted across selected limestone quarry operations, leading to the identification and evaluation of 70 individual risk factors. The results indicated that 2 risks (2.85%) were classified as very high, 2 risks (2.85%) as high, 45 risks (64.28%) as significant, 19 risks (27.14%) as possible, and 1 risk (1.42%) as acceptable. These findings underscore the complexity and potential danger inherent in quarry operations, where multiple risk factors coexist and interact. Consequently, strict adherence to occupational health and safety regulations by all employees is essential in mitigating the identified risks. Moreover, comprehensive and proactive safety strategies must be implemented to prevent workplace accidents and reduce the severity of their potential consequences. In addition to employee safety, limestone quarry operations also pose considerable environmental concerns. Therefore, several critical precautions should be taken into account during quarry operations. First, blasting activities should be continuously monitored to ensure technical compliance and safety. Second, all necessary environmental measures must be implemented to minimize the impact of blasting on surrounding ecosystems. Third, heavy machinery used within the quarry should undergo regular maintenance and safety inspections to ensure compliance with occupational safety standards. Fourth, emergency response teams should be established, and regular training sessions should be provided to employees to prepare them for potential emergency scenarios. Fifth, special attention must be given to complying with occupational health and safety regulations while considering the environmental footprint of quarry operations. In conclusion, this study emphasizes that a structured risk assessment process using methods such as Fine–Kinney can significantly contribute to identifying and prioritizing hazards in quarry operations. The implementation of corresponding control measures not only enhances workplace safety but also reduces environmental impacts. By combining technical supervision, equipment maintenance, employee training, and environmental stewardship, limestone quarry operators can foster a safer and more sustainable working environment. The findings of this study are intended to serve as a practical reference for improving risk management practices in the mining sector, particularly in limestone extraction industries where both human and environmental health are at stake.

Keywords: limestone quarry, risk assessment, fine–kinney method, occupational health and safety, environmental impact.

---

[1] Corresponding author

Investigation of Experimental and Theoretical Spectral Data of 2-Tridecyl-4,5-Dihydro-1H-Imidazole

Murat GENÇ[1], Zehra DOGRU ALPAYDIN [2], Vedat KARAHAN [3], Zuhal KARAGOZ GENÇ[4]

[1,2] Department of Chemistry, Faculty of Arts and Sciences, Adiyaman University, 02040, Adiyaman, Turkey
[3] Department of Chemical Engineering, Faculty of Engineering, Fırat University, 23119, Elazığ, Türkiye.
[4] Department of Pharmaceutical Technology, Faculty of Pharmacy, Adiyaman University, 02040, Adiyaman, Turkey
[1]mgenc23@gmail.com, [2]tugcedogru00@gmail.com, [3]vdtkrhn@gmail.com, [4]zuhalkaragoz23@gmail.com
[1](ORCID: 0000-0003-1224-4128), [2](ORCID: 0009-0004-9180-588),[3](ORCID: 0000-0002-0913-7826), [4](ORCID: 0000-0002-8847-9129)

Abstract

Imidazole and its derivatives represent one of the most fundamental classes of heterocyclic compounds in organic and medicinal chemistry. As a five-membered aromatic heterocycle containing two nitrogen atoms at the 1- and 3-positions, imidazole ($C_3H_4N_2$) exhibits remarkable amphoteric behavior, acting both as a weak base and as a weak acid. This unique duality enables imidazole to participate in a wide range of chemical and biochemical reactions, particularly proton-transfer processes, hydrogen bonding, and coordination to metal centers. As a result, the imidazole motif is frequently encountered in biological systems, such as in the amino acid histidine and the biogenic amine histamine, where it plays a critical role in enzymatic catalysis, buffering, and signaling pathways. The ubiquity of the imidazole nucleus in biomolecules and therapeutic agents underscores its pharmacological importance, with derivatives demonstrating antimicrobial, antifungal, anticancer, and neuroactive properties.

The present study focuses on the synthesis, structural characterization, and computational analysis of a long-chain substituted imidazoline derivative. Imidazolines are closely related to imidazoles, differing by the saturation of the 4,5-position of the ring, which confers additional flexibility in functionalization and alters the physicochemical properties of the compounds. Long-chain imidazoline derivatives are of particular interest because they can display surfactant-like properties, amphiphilicity, and enhanced lipophilicity, making them suitable for applications in both biological and industrial contexts. Furthermore, imidazoline frameworks are commonly investigated for their role in corrosion inhibition, antimicrobial activity, and as intermediates in drug discovery.

Synthesis of Long-Chain Imidazoline Derivative

In the first stage of this work, a long-chain 2-substituted imidazoline compound was successfully synthesized through a reaction involving myristoyl chloride and ethylenediamine under basic conditions in tetrahydrofuran (THF). The synthetic strategy was designed to introduce a hydrophobic long alkyl chain onto the imidazoline ring system, thereby modulating both the solubility and biological activity of the resulting compound. The reaction was carefully controlled to favor intramolecular cyclization, leading to the imidazoline core formation. The obtained compound was isolated, purified, and subsequently subjected to detailed structural characterization.

Experimental Characterization

The structural elucidation of the synthesized imidazoline derivative was performed using Fourier-transform infrared spectroscopy (FT-IR) and proton nuclear magnetic resonance spectroscopy (^{1}H-NMR).

FT-IR analysis confirmed the presence of characteristic functional groups, including N–H stretching vibrations, C=N stretching bands corresponding to the imidazoline ring, and absorptions related to the long-chain alkyl substituent.

^{1}H-NMR spectra provided insights into the proton environments within the molecule, demonstrating the expected chemical shifts associated with the imidazoline ring protons, as well as the methylene and terminal methyl groups of the alkyl chain. The splitting patterns and integration ratios further supported the proposed molecular structure.

These experimental techniques established a reliable foundation for confirming the successful synthesis of the target compound.

Theoretical Studies

---

[1] Corresponding author

In the second stage of the study, theoretical calculations were conducted using the Gaussian 09 software package, a widely utilized program for quantum chemical computations. The computational analyses aimed to complement and validate the experimental findings, while also providing additional insights into the electronic, structural, and spectroscopic properties of the synthesized compound.

- Theoretical ^{1}H-NMR spectra were simulated using density functional theory (DFT) with appropriate basis sets. The calculated chemical shifts closely matched the experimentally obtained values, reinforcing the accuracy of the structural assignment.

- Theoretical FT-IR spectra were also generated, with predicted vibrational frequencies showing excellent correlation with the experimental IR bands. Minor deviations were attributed to the well-known limitations of harmonic approximation in computational vibrational analysis.

- Thermodynamic parameters, including enthalpy (ΔH), Gibbs free energy (ΔG), and entropy (ΔS), were evaluated, providing valuable information about the stability of the compound and the feasibility of its formation under the experimental conditions employed.

- UV–Vis spectrum simulations were carried out to investigate the electronic transitions of the compound. The calculated absorption maxima corresponded to π–π^* and n–π^* transitions within the imidazoline ring system, as well as transitions influenced by the electron-donating and electron-withdrawing effects of the substituents.

Comparative Analysis

A significant finding of this study was the high degree of agreement between the experimental and theoretical results. Both ^{1}H-NMR and FT-IR data demonstrated close correspondence, with theoretical predictions effectively reproducing experimental spectra. This level of consistency confirms the reliability of the computational methods employed and highlights the value of combining experimental synthesis with quantum chemical approaches for comprehensive molecular characterization.

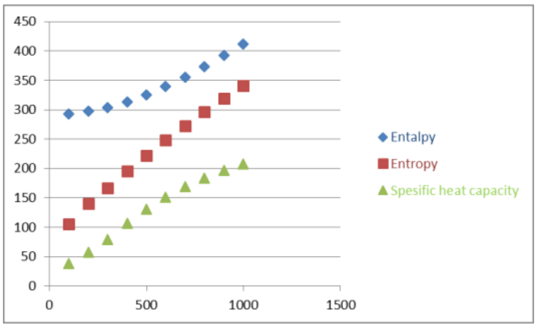
The thermodynamic and UV–Vis calculations further enriched the understanding of the physicochemical properties of the compound, while also suggesting its potential stability and electronic activity under physiological or application-relevant conditions. The integration of experimental and computational data thus provides a powerful framework for exploring structure–property relationships in heterocyclic compounds.

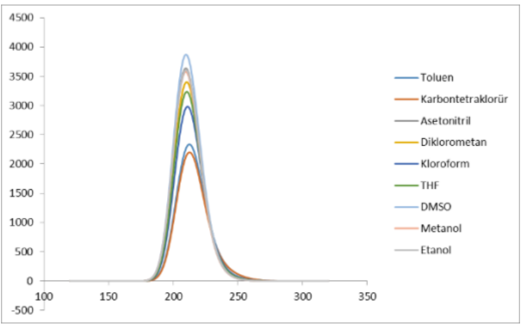
Implications and Conclusions

The successful synthesis and thorough characterization of a long-chain substituted imidazoline derivative represent a meaningful contribution to the expanding field of heterocyclic chemistry. The combined use of spectroscopic techniques (^{1}H-NMR and FT-IR) and quantum chemical methods (DFT-based Gaussian calculations) not only validated the structural identity of the compound but also provided complementary insights into its thermodynamic and spectroscopic behavior.

The consistency between experimental and theoretical findings underscores the effectiveness of such integrative approaches in modern chemical research. Moreover, the synthetic methodology employed here demonstrates a practical route to generating functionalized imidazoline derivatives with tailored properties. Given the amphiphilic nature conferred by the long alkyl chain, the compound synthesized in this study could be further investigated for potential applications in drug development, surfactant chemistry, and material science. Its imidazoline framework, coupled with lipophilic substitution, may endow it with promising biological activities, particularly in antimicrobial or anticancer contexts, while its physicochemical properties suggest possible roles in industrial formulations.

In conclusion, this study highlights the enduring relevance of imidazole and imidazoline derivatives in chemical and pharmaceutical research. By bridging experimental and theoretical approaches, a comprehensive understanding of molecular properties can be achieved, paving the way for rational design of novel compounds with desirable characteristics. The long-chain substituted imidazoline synthesized and analyzed herein thus serves not only as a model system for methodological validation but also as a potential candidate for future applied studies in medicinal chemistry and related disciplines.





Keywords: Imidazoline, Gaussian 09, DFT

References

[1] R. Thomas, M. Hossain, Y.S. Mary, K.S. Resmi, S Armakovic, S.J. Armakovic, A.K. Nanda, V.K. Ranjan, G. Vijayakumar, C.V. Alsenoy, “Spectroscopic analysis and molecular docking of imidazole derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations”, Journal of Moleculer Structure, 1158, 156-175, 2018.

[2] Gourona , K. L. Mapihanb , S. Camperosc , A. A. Farrac , V. Laira , A. Ringuedéa, M. Cassira , B. Diawaraa, “New insights in self-assembled monolayer of imidazolines on iron oxide investigated by DFT”, Applied Surface Science, 456, 437-444, 2018.

In Silico Molecular Docking of 2-Tridecyl-4,5-Dihydro-1H-Imidazole For Possible Treatment of Alzheimer's Disease

Murat GENÇ[1], Zehra DOGRU ALPAYDIN [2], Vedat KARAHAN [3], Zuhal KARAGOZ GENÇ[4]

[1,2] Department of Chemistry, Faculty of Arts and Sciences, Adiyaman University, 02040, Adiyaman, Turkey
[3] Department of Chemical Engineering, Faculty of Engineering, Fırat University, 23119, Elazığ, Türkiye.
[4] Department of Pharmaceutical Technology, Faculty of Pharmacy, Adiyaman University, 02040, Adiyaman, Turkey
[1]mgenc23@gmail.com, [2]tugcedogru00@gmail.com, [3]vdtkrhn@gmail.com, [4]zuhalkaragoz23@gmail.com
[1](ORCID: 0000-0003-1224-4128), [2](ORCID: 0009-0004-9180-588),[3](ORCID: 0000-0002-0913-7826), [4](ORCID: 0000-0002-8847-9129)

Abstract

Imidazole derivatives represent a fundamental class of heterocyclic compounds in pharmaceutical chemistry and have long been recognized for their versatile biological activities. The imidazole ring, a five-membered heterocycle containing two nitrogen atoms, exhibits remarkable electronic and structural properties that enable it to interact with a wide range of biological targets. Because of its ability to form hydrogen bonds, participate in π–π interactions, and coordinate with metal ions, the imidazole scaffold has been successfully incorporated into numerous bioactive molecules, making it a privileged structure in medicinal chemistry.

One of the most prominent features of imidazole derivatives is their broad pharmacological profile. Over the years, they have been investigated for antimicrobial, antifungal, anticancer, antiviral, anti-inflammatory, and neurological activities. Clinically approved drugs containing imidazole moieties highlight their importance in modern medicine. For example, metronidazole, a nitroimidazole derivative, is widely used as an antimicrobial agent in the treatment of protozoal infections and anaerobic bacterial diseases. Similarly, ketoconazole, an antifungal agent, exerts its therapeutic effect by inhibiting cytochrome P450 enzymes involved in ergosterol biosynthesis, thereby disrupting fungal cell membrane integrity. Beyond infectious diseases, imidazole derivatives have shown substantial potential in oncology. Several imidazole-based compounds act by inhibiting enzymes and signaling pathways critical for cancer cell proliferation, survival, and metastasis. Furthermore, imidazole derivatives are also incorporated into antidepressant and anxiolytic drugs, underscoring their importance in the treatment of central nervous system disorders. Collectively, these examples illustrate that imidazole derivatives are not confined to a single therapeutic area but instead provide a flexible chemical framework adaptable for multiple disease treatments.

Given this broad pharmacological relevance, there has been a growing interest in exploring novel imidazole derivatives with potential applications in neurodegenerative diseases, particularly Alzheimer's disease (AD). Alzheimer's disease is a progressive neurodegenerative disorder characterized by memory loss, cognitive impairment, and behavioral changes. It is currently the most common cause of dementia worldwide, with a growing prevalence due to the aging population. Pathologically, AD is associated with the accumulation of β-amyloid plaques, tau protein hyperphosphorylation, oxidative stress, and cholinergic system dysfunction. The limited number of effective therapeutic options for AD underscores the urgent need for novel compounds capable of modulating disease pathways.

In this context, the present study focuses on the imidazole derivative 2-Tridecyl-4,5-Dihydro-1H-Imidazole. The aim was to explore its electronic properties through quantum chemical calculations and to assess its potential activity against Alzheimer's disease via molecular docking studies. Such a computational approach provides valuable insights into the compound's structural, electronic, and pharmacological characteristics, serving as a foundation for further in vitro and in vivo studies.

The research was conducted in two main stages. In the first stage, quantum chemical calculations were performed using the Gaussian 09 software package. The calculated parameters included the HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) energy levels, electronegativity (χ), and chemical hardness (η). These parameters are essential for understanding the reactivity and stability of a molecule. The HOMO level indicates the ability of a molecule to donate electrons, while the LUMO level reflects its ability to accept electrons. The energy gap between HOMO and LUMO serves as a measure of molecular stability and electronic excitation potential; a smaller gap suggests higher reactivity and potential bioactivity. Electronegativity (χ) provides insights into the molecule's tendency to attract electrons, whereas chemical hardness (η) is a descriptor of resistance to charge transfer and reactivity. Together, these descriptors offer a comprehensive picture of the electronic structure of 2-Tridecyl-4,5-Dihydro-1H-Imidazole.

In the second stage, molecular docking simulations were carried out to investigate the compound's potential interactions with Alzheimer's-related biomolecular targets. Docking studies are a widely used computational tool in drug discovery because they provide information about how a small molecule fits into the active site of a target protein, the binding orientation, and the strength of the

---

[1] Corresponding author

interaction. In this study, docking calculations were focused on proteins that play a key role in the pathogenesis of Alzheimer's disease, such as acetylcholinesterase (AChE) and β-amyloid-related proteins. Inhibitors of AChE are of particular importance in Alzheimer's therapy, as they help increase acetylcholine levels in the brain, improving cognitive function and slowing disease progression.

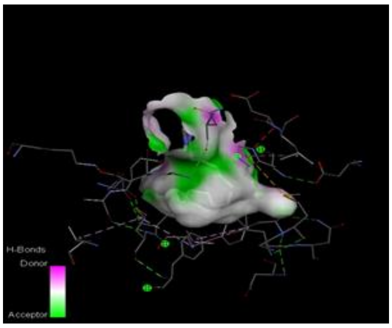
The computational results revealed significant findings. The HOMO–LUMO analysis indicated that 2-Tridecyl-4,5-Dihydro-1H-Imidazole possesses a favorable energy gap, suggesting an appropriate balance between stability and reactivity, which is advantageous for biological interactions. The calculated electronegativity value suggested that the compound has a reasonable tendency to attract electrons, which could facilitate interactions with enzyme active sites. Similarly, the chemical hardness parameter indicated that the compound exhibits moderate reactivity, a desirable feature for bioactive molecules as it implies the ability to interact with biological macromolecules without being overly reactive or unstable.

Molecular docking simulations further supported the compound's potential pharmacological activity. The docking results demonstrated that 2-Tridecyl-4,5-Dihydro-1H-Imidazole binds favorably to Alzheimer's-related targets, exhibiting strong binding affinities and favorable interaction profiles. Hydrogen bonding, van der Waals forces, and hydrophobic interactions were among the primary stabilizing interactions observed. The docking scores and binding orientations suggested that the compound could act as an effective modulator of the target proteins. Importantly, these computational results align with the hypothesis that imidazole derivatives may offer therapeutic potential in the treatment of neurodegenerative diseases.

The significance of this study lies not only in the promising activity of 2-Tridecyl-4,5-Dihydro-1H-Imidazole but also in the demonstration of the effectiveness of integrating quantum chemical analysis with molecular docking simulations. This multidisciplinary approach allows researchers to predict the pharmacological behavior of compounds before costly and time-consuming experimental testing, thereby accelerating the drug discovery process. By evaluating electronic properties alongside binding affinities, this study provides a more complete understanding of the compound's potential as a lead molecule in Alzheimer's research.

In conclusion, the results obtained suggest that 2-Tridecyl-4,5-Dihydro-1H-Imidazole is a promising candidate for further investigation as a potential therapeutic agent against Alzheimer's disease. The combination of favorable electronic properties and strong binding affinities to AD-related targets indicates that this compound may contribute to the development of new drugs for the treatment of neurodegenerative disorders. Future studies should include in vitro experiments to confirm enzyme inhibition activity, followed by in vivo evaluations to assess pharmacokinetics, bioavailability, and safety. Additionally, structural optimization and the synthesis of analogues could further enhance the biological activity and drug-like properties of this compound.

Ultimately, this research underscores the importance of imidazole derivatives in medicinal chemistry, not only in their established roles as antimicrobial and anticancer agents but also in their emerging potential in neurological disease therapy. By highlighting the activity of 2-Tridecyl-4,5-Dihydro-1H-Imidazole against Alzheimer's disease, this study adds to the growing body of evidence supporting heterocyclic chemistry as a cornerstone in modern drug discovery.



Keywords: Imidazoline, Gaussian 09, DFT

References

[1] Y. Nural, M. Gemili, N. Seferoglu, E. Sahin, M. Ulger, H. Sari, "Synthesis, crystal structure, DFT studies, acid dissociation constant, and antimicrobial activity of methyl 2-(4-chlorophenyl)-7a-((4-chlorophenyl)carbamothioyl)-1-

[2] oxo-5,5-diphenyl-3-thioxohexahydro-1H-pyrrolo[1,2-e]imidazole-6- carboxylate”, Journal of Moleculer Structure, 1160, 375-382, 2018.

[3] M. A. Quraishi, M. Z. A. Rafiquee, N. Saxena ve Sadaf Khan, “Inhibition of Mild Steel Corrosion in Presence of Fatty Acid Imidazolines in Hydrochloric Acid” Protection of Metals and Physical Chemistry of Surfaces, 44, 91–98, 2008.

Investigation of the Potential Activity of 3-((1H-benzotriazol-1-yl)methyl-4-ethyl-1H-1,2,4-triazol-5(4H)-thione Against MCF-7 and L1210 Cancer Cells

Murat GENÇ [1], Umut Ibrahim OGUZ [2], Vedat KARAHAN [3], Zuhal KARAGOZ GENÇ[4]

[1,2] Department of Chemistry, Faculty of Arts and Sciences, Adiyaman University, 02040, Adiyaman, Turkey
[3] Department of Chemical Engineering, Faculty of Engineering, Fırat University, 23119, Elazığ, Türkiye.
[4] Department of Pharmaceutical Technology, Faculty of Pharmacy, Adiyaman University, 02040, Adiyaman, Turkey
[1]mgenc23@gmail.com, [2]uioguz@gmail.com, [3]vdtkrhn@gmail.com, [4]zuhalkaragoz23@gmail.com
[1](ORCID: 0000-0003-1224-4128), [2](ORCID: 0000-0003-1993-8819),[3](ORCID: 0000-0002-0913-7826), [4](ORCID: 0000-0002-8847-9129)

Abstract

Cancer remains one of the most devastating health challenges of modern society and continues to represent the second leading cause of mortality worldwide, following cardiovascular diseases. Despite significant advances in medical science, diagnostics, and treatment strategies, the global incidence and death toll associated with cancer are still alarmingly high. This situation has directed increasing research efforts toward the discovery and development of novel anticancer agents with improved selectivity, reduced toxicity, and enhanced therapeutic potential. Among the various approaches, the design and synthesis of heterocyclic compounds have proven particularly fruitful, as heterocycles are well known for their diverse biological activities and broad pharmacological applications.

Within this framework, benzotriazole-based heterocyclic compounds and their nitrogen-containing derivatives have attracted considerable attention in recent years. Benzotriazole is a privileged scaffold in medicinal chemistry due to its ability to participate in strong π–π interactions, hydrogen bonding, and coordination with biological macromolecules, thereby conferring a wide spectrum of bioactivity. Compounds containing the benzotriazole moiety have been reported to exhibit antimicrobial, antifungal, antiviral, anti-inflammatory, and anticancer properties. This has made benzotriazole an important structural motif in the rational design of drug candidates.

In parallel, 1,2,4-triazole derivatives, which represent another important class of heterocyclic compounds, have been extensively studied in organic and medicinal chemistry. These compounds are known to act as fungicides, herbicides, antiepileptics, antitumor agents, and plant growth regulators. The triazole nucleus is particularly interesting because of its stability, hydrogen-bonding capacity, and ability to interact with biological targets such as enzymes and receptors. Moreover, 1,2,4-triazoles are often used as bioisosteres of amide or ester groups, thereby enhancing pharmacological activity, bioavailability, and metabolic stability. Importantly, several triazole-based drugs are already in clinical use, including antifungal agents such as fluconazole and itraconazole, highlighting the pharmaceutical significance of this heterocyclic system.

The combination of benzotriazole and triazole scaffolds within a single molecular framework offers an attractive strategy for designing hybrid compounds with potentially synergistic biological activities. This dual approach leverages the pharmacological advantages of both moieties, creating new opportunities for the development of potent anticancer agents. In this study, we focused on the synthesis of benzotriazole-substituted 1,2,4-triazole derivatives, their structural characterization, and theoretical evaluation of their anticancer potential against selected cancer cell lines.

The research was carried out in two main stages. In the first stage, the target compounds were synthesized through a series of organic transformations. Initially, Ethyl 2-(1H-benzotriazol-1-yl)acetate was obtained via the reaction of benzotriazole with ethyl bromoacetate. This ester derivative was subsequently reacted with hydrazine hydrate to yield 2-(1H-benzotriazol-1-yl)acetohydrazide. The hydrazide functionality is of particular interest in medicinal chemistry, as it can serve as a versatile precursor for the synthesis of heterocyclic systems with potential bioactivity.

Following this, the hydrazide was further transformed into a benzotriazole-substituted thiocarboamide derivative by reaction with ethyl isothiocyanate. The incorporation of a thiocarboamide group is notable because sulfur-containing heterocycles are frequently reported to enhance anticancer activity, often due to their ability to disrupt cellular redox balance or interact with biomolecular targets. Finally, the cyclization of this intermediate under basic conditions led to the formation of the desired benzotriazole-substituted 1,2,4-triazole derivative, completing the synthetic pathway. The entire series of reactions was performed using both conventional heating methods and microwave-assisted techniques. Microwave-assisted organic synthesis has emerged as a powerful approach in modern chemistry, offering advantages such as shorter reaction times, improved yields, and cleaner reactions. Comparing these two approaches allowed us to evaluate the efficiency and practicality of each method in synthesizing the target compounds.

---

[1] Corresponding author

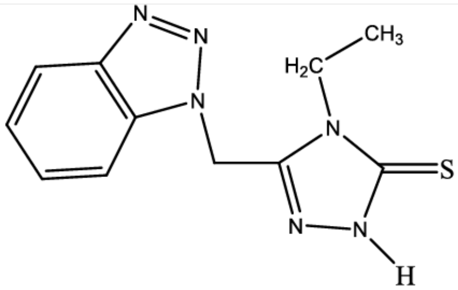
In the second stage of the study, theoretical and computational calculations were conducted to assess the electronic properties, molecular interactions, and potential anticancer activity of the synthesized compounds. Calculations were carried out using the Gaussian software package for quantum chemical studies and the AutoDock program for molecular docking simulations. Quantum chemical calculations provided insights into the structural stability, electronic distribution, and frontier molecular orbitals (HOMO–LUMO energy gap) of the compounds, which are critical parameters for predicting reactivity and biological activity.

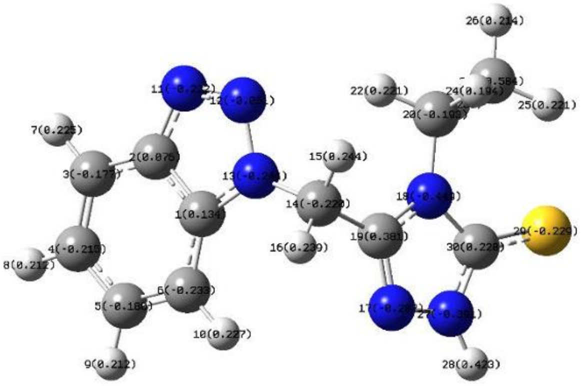
Molecular docking studies were then performed to evaluate the binding affinity of the synthesized triazole derivatives toward cancer-related biological targets. Docking simulations are widely used in drug discovery as they allow prediction of how small molecules interact with protein receptors at the molecular level. Our docking results suggested that the benzotriazole-substituted 1,2,4-triazole derivative exhibited favorable binding interactions with key active sites, supporting its potential as an anticancer agent. In particular, the compound showed promising activity against MCF-7 (human breast adenocarcinoma) and L1210 (mouse lymphocytic leukemia) cancer cell lines, both of which are widely used experimental models in cancer research. These findings suggest that the designed compounds may serve as potential leads for further biological evaluation and drug development.

The overall results of this study highlight several important aspects. First, the successful synthesis of benzotriazole-substituted 1,2,4-triazole derivatives demonstrates the feasibility of combining two pharmacologically significant heterocyclic systems into a single framework. Second, the use of microwave-assisted synthesis proved to be a practical alternative to conventional methods, offering advantages in terms of reaction efficiency. Third, theoretical calculations and molecular docking studies provided valuable preliminary evidence supporting the anticancer potential of the synthesized compounds, specifically against breast and leukemia cancer models.

The significance of this research lies not only in the synthesis of new heterocyclic derivatives but also in the demonstration of an integrated approach that combines synthetic chemistry with computational modeling. Such a multidisciplinary strategy is increasingly recognized as essential in modern drug discovery, where computational predictions can guide experimental design, reduce the cost of trial-and-error experimentation, and accelerate the identification of promising candidates.

In conclusion, the benzotriazole-substituted 1,2,4-triazole derivative synthesized in this study represents a promising scaffold for further anticancer research. The encouraging docking results against MCF-7 and L1210 cancer cell lines warrant additional in vitro and in vivo studies to validate the computational predictions. Furthermore, structural modifications and optimization strategies could be applied to enhance activity, improve pharmacokinetic properties, and minimize potential toxicity. Ultimately, the insights gained from this work contribute to the growing body of knowledge on heterocyclic chemistry in drug discovery and provide a foundation for the future development of novel anticancer therapeutics.





Keywords: Benzotriazole, Gaussian 09, DFT

References

[1] Patel, J. S, Garg, C. S., and Sen, D. J., (2012), "Synthesis of Novel N Substituted 2(1H-Benzotriazol-1-yl)-Acetohydrazide Derivatives as Antimicrobial agents", Int. J. Drug Dev. & Res., 4(2): 322-329.

[2] Srivastava, S.K., Srivastava, S. and Srivastava, S.D., (2002), Synthesis of 5Arylidene-aryl-3-(1,2,4-triazoloacetamidyl)-1,3-thiadiazol-4-ones as antibacterial, antifungal, analgesic and diuretic agents. Indian J Chem, 41B.

[3] Srivastava, S.K., Srivastava, S. and Srivastava, S.D., (2002), Synthesis of new 1,2,4triazolo-thiadiazoles and its 2-oxoazetidines as antimicrobial, anticonvulsant and anti-inflammatory agents. Indian J Chem. 41B, 2357-2363.

Behavior of Sodium Bentonite in Acidic and Alkaline Environments: Modeling Filtrate Properties with Machine Learning

Fatih KAYA[1], Umay HALİSDEMİR[2], Şeyda TAŞAR[3], Beyda TAŞAR[4], Gülbeyi DURSUN[5]

[1,3,5] Chemical Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[2] Environmental Engineering Department, Engineering Faculty, Atatürk University, Elazığ, TURKEY.
[4]Mechatronic Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[1]fatihkaya@firat.edu.tr, [2]umayhalisdemir@gmail.com, [3]sydtasar@firat.edu.tr, [4]btasar@firat.edu.tr, [5]gdursun@firat.edu.tr
[1](ORCID: 0000-0002-4063-8362), [2](ORCID: 0000-0002-0673-6233), [3](ORCID: 0000-0003-3184-1542), [4](ORCID: 0000-0002-2771-3524), [5](ORCID: 0000-0001-7788-9766)

Abstract

Colemanite ore may contain montmorillonite-type clay minerals in the range of 5-10% depending on its mineralogical composition. During the boric acid production process, clay minerals in the ore interact with sulfuric acid, increasing the impurity value of the solution medium and increasing the acid consumption of the process. In this direction, understanding the behavior of clay minerals in acidic, alkaline, and neutral conditions is very important in terms of understanding and controlling the impurity formation in the boric acid production process. For this reason, in this study, sodium bentonite was treated with solution mediums at different pH values and then the solution medium was analyzed chemically and physicochemically to interpret the clay behavior.

In the studies conducted, the behavior of clay minerals (sodium bentonite) under different pH and impregnation time conditions was examined in detail and the effects of process parameters on the filtrate were evaluated by analytical and instrumental means. As a result of the analysis carried out with the pH drift method, the pHzpc value of sodium bentonite was determined as 8.5. This result shows that in alkaline environments with pH > pHzpc, the surfaces are negatively charged, dispersion stability increases, and the amount of suspended solid particles increases, causing filtration difficulties. In viscosity measurement experiments carried out at 25°C, it was observed that the viscosity was in the range of 0.9–1.8 cP in acidic environments, increased to 4–5 cP in pH 3–5 environments, and reached up to 6.6 cP in pH 7–9. Filtrate turbidity (NTU) analyses confirm that the filtrates turn yellow and the amount of suspended solid particles increases as the pH increases. As a result of the particle size distribution analysis of the filtrates, it was concluded that while acidic environments (low pH) form larger and easily separable particle groups, basic environments (high pH) increase the dispersion and stability of small particles, making separation difficult. FTIR analysis results showed that the structure of sodium bentonite continues to be basically preserved under different pH and water quality conditions and there is no significant change in its chemical structure. This shows that the changes in viscosity and turbidity observed in the dispersion medium are mainly due to physicochemical parameters such as surface charge balance and particle size distribution. As a result, it was understood that keeping the reactor pH in the range of pH 2–4 will increase the ease of filtration by reducing the amount of suspended solid particles, while in alkaline environments, temperature and pH control should be optimized together to prevent filtration difficulties due to suspended particles and viscosity increase.

Various machine learning algorithms were used to further evaluate the filtrate properties (ICP analysis data, pH_f, conductivity). Models created with methods such as Boosted Trees, Random Forest, Bagged Trees, Gaussian Process Regression (GPR), Support Vector Machines (SVM), and Linear Regression were comparatively evaluated for their success in predicting pH_f, conductivity, and metal ion concentrations in solution. Especially Boosted Trees and GPR models achieved high accuracy values such as $R^2 > 0.95$ for many output variables. For example, for conductivity (Out2) in the Boosted Trees model, $R^2 = 0.9998$, and for Si concentration (Out6) $R^2 = 0.9939$ were determined. Partial dependency analyses were used to interpret the model's prediction mechanisms and revealed that the effects of pH and time on the output variables were decisive. In addition, correlations and ionic interactions between elements such as Na, Ca, Fe, and Si were determined graphically and the complex interaction network in the solution was interpreted. It was concluded that especially for ions such as Al and Mg, Random Forest and Boosted Trees algorithms exhibited superior performance.

Keywords: sodium bentonite, pH behavior, filtrate properties, machine learning, FTIR, ICP, zeta sizer, pHzpc

---

[1] Corresponding author

Modeling of Biochar Production Process Efficiency from Tea Pulp and Almond Outer Shell Using Machine Learning Methods

Şeyda TAŞAR[1] , Beyda TAŞAR[2], Yalew Woldeamanuel SITOTAW [3]

[1]Chemical Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[2]Mechatronic Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[3]Chemical Engineering Department, Engineering Faculty, Addis Ababa Science and Technology University, Addis Ababa, Etiyopya
[1]sydtasar@firat.edu.tr, [2]btasar@firat.edu.tr, [3]yalew.woldeamanuel@aastu.edu.et
[1](ORCID: 0000-0003-3184-1542), [2](ORCID: 0000-0002-2771-3524),[3](ORCID: 0000-0003-2512-8898)

Abstract

In recent years, the importance of renewable energy sources has increased globally in terms of energy supply security, environmental sustainability, and combating climate change. Within the scope of renewable energy sources, the energy production process from biomass sources has emerged as an environmentally friendly alternative to fossil fuels due to a series of advantages, including the rapid renewability of the raw material, its carbon-neutral properties, and its local availability [1–3]. Waste biomass sources used in bioenergy production include organic waste such as plant and animal waste, agricultural by-products and residues, food industry factory waste, municipal waste, and forest waste (pruning, cutting waste, etc.) [1–2]. Biomass sources have significantly lower sulfur and nitrogen content compared to fossil energy sources, resulting in lower NO_x and SO_x emissions during combustion processes [4–5]. Because biomass resources are carbon neutral, they do not cause CO_2 emissions. This way, they minimize environmental problems and contribute significantly to preventing global warming and acid rain, which are among the goals of the Kyoto Protocols [6]. Turkey has a high agricultural production potential and, due to its large forest areas, also possesses significant biomass reserves. The Biomass Energy Potential Atlas (BEPA), published by the Ministry of Energy and Natural Resources of the Republic of Turkey, reports that approximately 100 million tons of biomass waste is generated annually in our country [7]. Furthermore, it is known that a significant portion of this biomass waste cannot be recycled, resulting in no economic or environmental benefits. The reuse of waste biomass has become a necessity for our country for energy production and sustainability [8-9].

Thermochemical processes, especially pyrolysis processes, provide significant advantages in the conversion of primary biomass resources into energy. Pyrolysis, which can also be defined as the controlled degradation of organic matter at high temperatures in an inert atmosphere, is a process that results in the formation of biochar, bio-oil, and gas products [10]. The distribution efficiency and product composition of biochar, bio-oil, and biogas products formed as a result of pyrolysis can vary depending on many parameters. These include pyrolysis temperature (HTT), heating rate (HR), nitrogen flow rate (FR), particle size of the waste biomass source, residence time, and biomass composition [10–12]. The chemical structure of biomass sources, such as cellulose, hemicellulose, and lignin ratios, as well as short-term analysis results (moisture, volatile matter, ash, and fixed carbon) and final analysis data (amounts of carbon, hydrogen, nitrogen, oxygen, and sulfur), have a significant impact on this process [8, 11]. Pyrolysis is a variable and nonlinear thermal transformation process and, therefore, is quite difficult to model using classical statistical methods. In recent years, the use of machine learning techniques to model pyrolysis processes has become quite popular. This is because researchers have demonstrated that regression models such as Support Vector Machines (SVM) [14], Artificial Neural Networks (ANN) [15], Decision Trees (DT), and Random Forests (RF) [16] can model the thermal conversion efficiency of biomass with high accuracy. In addition, ML-based approaches also produce successful results in high calorific value (HHV) estimation and crop yield modeling [17].

In this study, biochar was produced from two biomass sources (tea pulp and almond outer shell), which are generated in large quantities as waste as a result of agricultural and industrial activities in Türkiye. Biochar production efficiency was modeled using machine learning techniques as a function of pyrolysis variable parameters. In the study, the effects of temperature, retention time, heating rate, and nitrogen flow rate were evaluated as pyrolysis variable parameters. The experimental data obtained as a result of the study carried out under varying conditions were used as datasets and modeled using machine learning methods. The data was analyzed using Linear, Lasso, Ridge, ElasticNet, and Deep Neural Network (DNN) regression models. The dataset was normalized during the modeling process, and the HoldOut method was applied, with an 80% training and 20% test data separation. Performance evaluations indicated that classical linear models (Linear, Ridge) were inadequate, especially in extreme values. In contrast, Lasso and ElasticNet models modeled the study data with lower error and higher explanatory power. The best performance result was achieved with the DNN model with $R^2 = 0.9937$, RMSE = 5.0123, MAE = 3.44. Single and multivariate partial dependency analyses confirmed that carbonization temperature and volatile matter ratio are the main parameters affecting biochar yield for both biomass types. It was determined that biochar yield decreased significantly at temperatures above 600°C and raw material compositions above 50% volatile ratio, while liquid and gas product yields increased.

---

[1] Corresponding author

The study also found that biochar yield was maximum in the pyrolysis temperature range of 400–500°C and in moderate retention time conditions. Overall, the study demonstrated the applicability of data-driven decision-making processes in biochar production. It has been proven that machine learning modeling approaches can have strategic importance for sustainable waste management and energy conversion systems.

Keywords: biochar, tea pulp, almond outer shell, biochar yield, pyrolysis, machine learning

References

[1] P. McKendry, Energy production from biomass (Part I): overview of biomass, Bioresour. Technol. 83 (2002) 37–46.
[2] P. McKendry, Energy production from biomass (part 2): conversion technologies, Bioresour. Technol. 83 (2002) 47–54.
[3] Ş. Taşar, Developing a new model equation between proximate compositions of biomass resources and upper heat values and investigation of the model equation’s success, Artvin Coruh Univ. J. For. Fac. 22 (1) (2021) 42–51.
[4] J.F. Gonzalez, C. Gonzalez-Garcıa, A. Ramıro, J. Gonzalez, E. Sabıo, J. Ganan, M. Rodrıguez, Combustion optimization of biomass residue pellets for domestic heating with a mural boiler, Biomass Bioenergy 27/2 (2004) 145–154.
[5] Ş. Taşar, Thermal conversion behavior of cellulose and hemicellulose fractions isolated from tea leaf brewing waste: kinetic and thermodynamic evaluation, Biomass. Conv. Bioref. (2021), https://doi.org/10.1007/s13399-021-01697-2.
[6] B.M. Jenkins, L.L. Baxter, J.T.R. Miles, T.R. Miles, Combustion properties of biomass, Fuel Process. Technol. 54 (1998) 17–46.
[7] BEPA-T. C. Ministry of Energy and Natural Resources General Directorate of Energy Affairs, Biomass Energy Potential Atlas, https://bepa.enerji.gov.tr/.
[8] M. Tan, H. Li, Z. Huang, Z. Wang, R. Xiong, S. Jiang, J. Zhang, Z. Wu, C. Li, L. Luo, Comparison of atmospheric and gas-pressurized oxidative torrefaction of heavymetal-polluted rice straw, J. Clean. Prod. 28 (2021), 124636.
[9] Tashtoush G. Al-Widyan, M. Hamasha, Combustion and emissions of pulverized olive cake in a tube furnace, Energy Convers. Manag. 47 (11–12) (2006) 1588–1596.
[10] S. Yaman, Pyrolysis of biomass to produce fuels and chemical feedstocks, Energy Convers. Manag. 45 (2004) 651–671.
[11] J. Li, Y.Q. Chen, H.P. Yang, D.C. Zhu, X. Chen, X.H. Wang, H.P. Chen, Correlation of feedstock and bio-oil compound distribution, Energy Fuels 31 (7) (2017) 7093–7100.
[12] A. Oasmaa, Y. Solantausta, V. Arpiainen, E. Kuoppala, K. Sipila, Fast pyrolysis biooils from wood and agricultural residues, Energy Fuels 24 (2) (2010) 1380–1388.
[13] H.L. Cao, Y. Xin, Q.X. Yuan, Prediction of biochar yield from cattle manure pyrolysis via least squares support vector machine intelligent approach, Bioresour. Technol. 202 (2016) 158–164.
[14] Y.F. Sun, L.N. Liu, Q. Wang, X.Y. Yang, X. Tu, Pyrolysis products from industrial waste biomass based on a neural network model, J. Anal. Appl. Pyrolysis 120 (2016) 94–102.
[15] S.R. Naqvi, Z. Hameed, R. Tariq, S.A. Taqvi, I. Ali, M.B.K. Niazi, T. Noor, A. Hussain, N. Iqbal, M. Shahbaz, Synergistic effect on co-pyrolysis of rice husk and sewage sludge by thermal behavior, kinetics, thermodynamic parameters and artificial neural network, Waste Manag. 85 (2019) 131–140.
[16] J.K. Xing, K. Luo, H.O. Wang, Z.W. Gao, J.R.A. Fan, comprehensive study on estimating higher heating value of biomass from proximate and ultimate analysis with machine learning approaches, Energy 188 (2019), 116077.
[17] Q. Tang, Y. Chen, H. Yang, M. Liu, H. Xiao, Z. Wu, H. Chen, S.R. Naqvi, Prediction of bio-oil yield and hydrogen contents based on machine learning method: effect of biomass compositions and pyrolysis conditions, Energy Fuels 34 (9) (2020) 11050–11060.

The Role of Activated Carbon in Supercapacitor Technology

Mohamad Obeid ALABİAD[1], Şeyda TAŞAR[2], Neslihan DURANAY[3]

[1,2,3] Chemical Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[1]obeid.alabiad@gmail.com, [2]sydtasar@firat.edu.tr, [3]nduranay@firat.edu.tr
[1](ORCID: 0000-0000-0000-0000), [2](ORCID:0000-0003-3184-1542), [3](ORCID:0000-0001-7259-1864)

Abstract

As the world shifts toward more sustainable and high-performance energy solutions, supercapacitors are emerging as a powerful alternative to conventional energy storage systems [1,2]. With their remarkable attributes—high power density, rapid charge and discharge capability, long cycle life, and operational safety—supercapacitors [3] are increasingly being used in applications ranging from portable electronics to electric vehicles and smart grids [4].

The overall performance of a supercapacitor is heavily influenced by the materials used for its electrodes and electrolytes [5]. Among electrode materials, activated carbon stands out due to its exceptionally high surface area, tunable pore structure, excellent electrical conductivity, and strong chemical and thermal stability [6,7]. These properties can be tailored by selecting appropriate biomass precursors and optimizing activation conditions, allowing for versatile and efficient material design [8,9].

This paper presents a comprehensive overview of biomass-derived precursors for the production of activated carbon, highlighting both physical activation methods (such as steam and CO_2) and chemical techniques (including KOH and H_3PO_4 treatments). The resulting carbon materials are evaluated based on their surface morphology, porosity, and electrochemical performance. The paper also explores the underlying mechanisms of electric double-layer capacitors (EDLCs), pseudocapacitors, and hybrid supercapacitors. Particular attention is given to the interactions at the electrode–electrolyte interface, examining how different electrolyte types—aqueous, organic, ionic liquids, and biomass-based—impact energy density, power output, and long-term stability.

Recent literature increasingly points to the value of converting agricultural and industrial biomass waste into functional carbon materials. These renewable sources offer an eco-friendly, low-cost, and sustainable pathway to next-generation energy storage technologies—supporting the global transition toward clean and resilient energy systems.

Keywords: supercapacitor, activated carbon, biomass, energy storage, electrode materials

References

[1] Olabi, A. G., Abbas, Q., Al Makky, A., & Abdelkareem, M. A. (2022). Supercapacitors as next generation energy storage devices: Properties and applications. Energy, 248, 123617.
[2] Aghmadi, A., & Mohammed, O. A. (2024). Energy storage systems: technologies and high-power applications. Batteries, 10(4), 141.
[3] Gopi, C. V. M., Alzahmi, S., Narayanaswamy, V., Vinodh, R., Issa, B., & Obaidat, I. M. (2025). Supercapacitors: A promising solution for sustainable energy storage and diverse applications. Journal of Energy Storage, 114, 115729.
[4] Amer, M., Elmojarrush, A., & Alsosi, A. (2025). Materials of Supercapacitor: Applications and Developments. Int. J. Electr. Eng. and Sustain., 01-18.
[5] Sowbakkiyavathi, E. S., Arunachala Kumar, S. P., Maurya, D. K., Balakrishnan, B., Guo, J. Z., & Subramania, A. (2024). Research progress in the development of transition metal chalcogenides and their composite-based electrode materials for supercapacitors. Advanced Composites and Hybrid Materials, 7(4), 130.
[6] Sun, H., Li, J., Liang, W., Gong, X., Jing, A., Yang, W., ... & Ren, S. (2024). Porous organic polymers as active electrode materials for energy storage applications. Small Methods, 8(8), 2301335.
[7] Czagany, M., Hompoth, S., Keshri, A. K., Pandit, N., Galambos, I., Gacsi, Z., & Baumli, P. (2024). Supercapacitors: An efficient way for energy storage application. Materials, 17(3), 702.
[8] Sagadevan, S., Balakrishnan, T., Rahman, M. Z., Soga, T., Randriamahazaka, H., Kakavandi, B., & Johan, M. R. (2024). Agricultural biomass-based activated carbons for efficient and sustainable supercapacitors. *Journal of Energy Storage*, *97*, 112878.
[9] Kadyan, P., Grover, S., & Sharma, R. K. (2024). Review on biomass derived activated carbons as electrochemical electrode material for supercapacitor device. Current Materials Science, 17(2), 116-134.

Thermal Convection Zone Detection for Glider Soaring Control via Seven-Class Cloud Type Classification Using Swin Transformer on Ground-Based Images

Beyda TAŞAR[1] , Orhan YAMAN[2], Ahmet Burak TATAR[3], Oğuz YAKUT[4]

[1,3,4] Mechatronic Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[2]Department of Digital Forensics, Faculty of Technology, Firat University, Elazig, TURKEY.
[1]btasar@firat.edu.tr, [2]orhanyaman@firat.edu.tr, [3] atatar@firat.edu.tr, [4]oyakut@firat.edu.tr
[1](ORCID: 0000-0002-4689-8579), [2](ORCID: 0000-0001-9623-2284),[3](ORCID: 0000-0001-5848-443X) ,[4](ORCID: 0000-0002-0986-1435)

Abstract

Clouds, as dynamic and visual manifestations of atmospheric processes, are key indicators in both weather forecasting and the identification of thermal convection regions. Their types, formations, and altitudes carry critical information about vertical air movements, moisture content, and heat distribution in the atmosphere. Among these, cumulus and cumulonimbus clouds—typically formed by rising warm air masses due to surface heating—are particularly significant as they mark active thermal zones. These thermals are not only crucial in meteorology but also play a pivotal role in the field of aeronautics, especially in glider soaring control, where pilots rely on naturally occurring updrafts to maintain altitude and prolong flight without engine propulsion.

The primary aim of this study is to develop a robust and intelligent computer vision framework capable of automatically detecting thermal convection indicators—specifically cumulus-related cloud formations—from ground-based images. This is pursued with the overarching goal of supporting real-time soaring decision systems for glider aircrafts. Unlike powered aircrafts, gliders rely heavily on environmental cues such as thermal lift, which is inherently invisible but can be inferred through visual indicators like cloud structures. Currently, most soaring decisions are made manually by experienced pilots based on visual observation. However, this method is highly subjective and can be unreliable under variable atmospheric lighting or visibility conditions. An AI-powered visual detection tool trained to recognize thermal-relevant cloud types can therefore significantly enhance flight safety, energy efficiency, and autonomous soaring capabilities.

To address this need, we utilized the publicly available Cloud Type Classification 3 dataset from Kaggle, which consists of 960 labeled ground-based sky images categorized into seven distinct classes: cirriform, high cumuliform, stratocumulus, cumulus, cumulonimbus, stratiform, and clear sky. This comprehensive dataset provides a rich source of atmospheric visual patterns necessary for deep learning-based classification tasks. The study pipeline began with exploratory data analysis (EDA) to examine image characteristics, class distributions, and resolution diversity. All images were then uniformly resized to 224×224 pixels to conform with the input requirements of the deep learning model. To improve model generalization and performance, data augmentation techniques such as random rotation, shifting, zooming, and flipping were applied. The image labels were numerically encoded using LabelEncoder, and the dataset was randomly split into training and testing sets. For the classification task, we adopted the Swin Transformer architecture—a state-of-the-art hierarchical vision transformer known for its powerful representation capacity and ability to capture fine-grained spatial features. The model was trained using the CrossEntropyLoss function and optimized via the Adam algorithm. The evaluation metrics included precision, recall, F1-score, and class-wise accuracy, providing a comprehensive understanding of the model's performance.

Results indicated that the model achieved high classification performance, particularly for thermally relevant cloud types such as cumulus and cumulonimbus. Even in classes with fewer samples, the model demonstrated competitive performance, although some false positives were observed, suggesting the potential benefit of class balancing or data resampling in future work. The average classification accuracy across all seven classes was recorded at 95%, confirming the model's efficacy in diverse sky conditions. The model achieved a precision of 0.98, a recall of 0.98, and an F1-score of 0.98 for the cumulus category, indicating a highly successful identification of cumulus clouds within the dataset. This result is especially significant considering the role of cumulus formations as visual markers of active updrafts, which are essential for maintaining altitude in unpowered flight. The model's ability to consistently recognize cumulus structures, despite variations in lighting, shape, and background conditions, suggests a strong internal representation of the morphological and textural features unique to this cloud type. Given that cumulus clouds typically form between 500 and 2000 meters as a result of surface heating, their accurate detection aligns directly with the goal of supporting real-time glider navigation through thermal exploitation. Moreover, the high recall value in this class ensures that very few thermally active clouds are missed, which is critical for flight safety and efficiency. These findings validate the applicability of vision transformer architectures like Swin Transformer in operational meteorology and autonomous aviation,

---

[1] Corresponding author

where the accurate and timely recognition of cumulus clouds can serve as a decision-support mechanism for dynamic soaring strategies.

In conclusion, this study demonstrates the viability of deep learning-based cloud type classification as a reliable tool for atmospheric analysis and decision support in glider aviation. The proposed Swin Transformer model successfully learns the morphological patterns of clouds and enables visual detection of thermally active zones, providing a foundational step toward intelligent flight control systems in unpowered aerial platforms.

Keywords: Cloud classification, Swin Transformer, glider flight, thermal convection, cumulus clouds, image processing, deep learning.

FireStageNet: A Transformer-Based Deep Learning Approach for Image-Based Fire Stage Classification

Beyda TAŞAR[1] , Orhan YAMAN[2], Ahmet Burak TATAR[3], Alper Kadir TANYILDIZI[4]

[1,3,4] Mechatronic Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[2]Department of Digital Forensics, Faculty of Technology, Firat University, Elazig, TURKEY.
[1]btasar@firat.edu.tr, [2]orhanyaman@firat.edu.tr, [3] atatar@firat.edu.tr, [4] atanyildizi@firat.edu.tr
[1](ORCID: 0000-0002-4689-8579), [2](ORCID: 0000-0001-9623-2284),[3](ORCID: 0000-0001-5848-443X) ,[4](ORCID: 0000-0003-3324-5445)

Abstract

Wildfires and structural fires represent a growing global threat, exacerbated by climate change, prolonged drought conditions, and the increasing human encroachment into wildland-urban interfaces. These fires not only result in tragic loss of life and irreversible ecological damage, but also incur significant economic costs through the destruction of infrastructure, agricultural assets, and natural resources. According to global disaster databases, fire-related incidents have caused billions of dollars in losses and displaced thousands of people annually. Therefore, the development of advanced fire detection technologies has become a critical focus for both the research community and public safety agencies.

While traditional fire detection systems primarily rely on smoke sensors, infrared detectors, or human observation, recent advancements in computer vision and deep learning have opened up promising avenues for visual fire analysis. However, most existing image-based fire detection models operate on a binary classification paradigm, identifying whether a fire exists or not. This binary approach lacks contextual awareness of the fire's progression, which is vital for emergency response planning, resource allocation, and early intervention. Particularly in applications such as unmanned aerial vehicles (UAVs), robotic firefighting systems, and early-warning monitoring platforms, the ability to differentiate no_fire, start_fire, and fire stages can significantly improve decision-making precision. To address this gap, we propose FireStageNet, a novel deep learning architecture designed to perform three-stage fire classification using 804 RGB images. The model architecture is grounded in the transformer paradigm and incorporates two key innovations: (1) a Patch Embedding layer that tokenizes image regions for spatially localized processing, and (2) a specially designed Fire-Aware Attention block that emphasizes features specific to fire characteristics such as smoke diffusion, flame contours, and thermal coloration. Unlike standard Vision Transformer (ViT) blocks, the attention mechanism in FireStageNet is optimized for fire-specific saliency, enabling it to discern subtle cues in early-stage fires.

The model was trained using the PyTorch framework on a curated fire dataset from Kaggle, featuring labeled instances of all three fire stages. Data augmentation techniques, including color jittering and horizontal flipping, were applied to improve generalization. The dataset was split into 80% training and 20% validation sets. The model was trained for 50 epochs using the AdamW optimizer and cross-entropy loss with label smoothing, promoting stability and robustness.

Experimental results reveal that FireStageNet achieves an overall classification accuracy of 88%, with a macro-averaged F1-score of 0.85. Class-wise F1-scores were recorded as 0.92 (fire), 0.90 (no_fire), and 0.74 (start_fire). While early-stage fire detection remains a challenge due to its visual ambiguity, ROC-AUC values exceeding 0.90 for all classes affirm the model's strong discriminative capability. These findings demonstrate that FireStageNet can serve as an effective tool in real-time, embedded fire detection systems for intelligent disaster response.

Keywords: fire stage classification, vision transformer, fire-aware attention, deep learning.

---

[1] Corresponding author

Photocatalysis Applications of MnOx-Decorated Biphasic Nanostructures: Methylene Blue Model

Sena Nur KÖKSAL[1] , Anıl KARATEPE [2], Ayşegül Ülkü METİN [3*]

Department of Chemistry, Faculty of Engineering and Natural Sciences, Kırıkkale University, Kırıkkale, Türkiye
[1]senanurkoksal@kku.edu.tr, [2]210102017@kku.edu.tr, [3]aumetin@kku.edu.tr
[1](ORCID: 0009-0004-9404-9004), [2](ORCID: 0009-0009-8767-8888),[3](ORCID: 0000-0001-8494-601X)

Abstract

Introduction: The rapid increase in industrial discharges and marine pollutants has brought environmental issues to a critical point, endangering aquatic biodiversity. Dyes released in industrial wastewater severely disrupt the chemical balance of aquatic systems, intensifying toxic effects. In dye-contaminated waters, photosynthetic marine plants are damaged, heavy metals compromise fish health, and certain textile dyes that infiltrate drinking water pose serious risks to human health. Methylene blue (MB) hinders sunlight penetration when released into water, thereby making underwater life difficult and causing environmental problems like marine mucilage. Rapid growth in industries such as textiles has increased the volume of dye-containing wastewater. Conventional treatment methods (chemical or bioligical treatments) are usually insufficient to remove these organic pollutants. Therefore, it is important to develop effective, economical, and sustainable treatment technologies that protect the environment and human health.

Photocatalytic processes, driven by light energy, have emerged as promising solutions owing to their high efficiency, low energy requirements, and environmental sustainability. However, the performance of photocatalysts strongly depends on factors like surface area, structural integrity, light absorption ability, and efficient charge transport. Nanomaterials attract attention due to their high surface area and tunable physicochemical properties. Boron nitride (BN) serves as an effective support material owing to its durability and large surface area, while manganese oxides (MnOx) are well-suited for photocatalytic applications due to their favorable crystal structure and strong oxidative potential. In this study, MnOx nanoparticles were synthesized on BN nanosheets through an environmentally friendly approach. *Stevia rebaudiana* extract, a plant-based reducing agent, was used to minimize the use of toxic chemicals during synthesis. The photocatalytic activity of the resulting nanocomposites was evaluated using methylene blue as a model pollutant, and their potential for wastewater treatment was assessed. This green synthesis method offers a promising route for the development of eco-friendly and efficient materials for environmental remediation.

Materials and Methods: MnOx were immobilized onto exfoliated and modified BN nanoparticles via adsorption, then converted to their hydroxylated forms through a green synthesis approach. Subsequent calcination yielded the MnOx/BN nanocomposite. For this purpose, firstly BN was exfoliated by HCl acid solution (0.35 M) and ethanol. In surface modification, functional groups capable of binding Mn (II) ions were introduced onto the BN surface. The modified BN was immersed in an aqueous solution containing Mn (II) ions at an appropriate concentration to immobilize Mn (II) ions on the surface. Subsequently, Mn (II) ions were reduced to MnOx nanoparticles on the surface using *Stevia rebaudiana* plant extract as a natural reducing agent. The resulting material was then calcined at 200 °C for 4 hours in an air atmosphere to obtain the MnOx/BN nanocomposite. Material characterization was performed using SEM and TEM for morphology and particle size, XRD for crystal structure, and FTIR for surface functional group analysis. Optical properties and photocatalytic activity of the BN/MnOx nanostructures were monitored by UV-Vis spectroscopy. Photocatalytic activities were tested using MB solutions at specified concentrations. MB solution was added to the reaction medium containing MnOx/BN nanocomposite, and the decolorization process was monitored over time under different light sources (UV and visible light) using UV-Vis spectroscopy. Parameters such as pH, temperature, and reaction time were systematically varied to determine optimal working conditions. Additionally, control experiments were conducted using pure BN and only MnOx. Photocatalytic activity was evaluated using MB solutions of specified concentrations. The MB solution was mixed with the MnOx/BN nanocomposite, and decolorization was monitored over time under UV (λ=365 nm) UV-Vis spectroscopy. Key parameters including pH, temperature, and reaction time were varied to identify optimal conditions. Control experiments with modified BN alone were also performed.

Conclusion: In this study, MnOx/BN nanostructures were successfully synthesized via a green synthesis route and comprehensively characterized. The resulting MnOx-decorated biphasic nanostructures exhibited enhanced photocatalytic performance, enabling the rapid and efficient degradation of MB. Among the nanostructures synthesized by immobilizing Mn (II) onto modified BN at different pH levels (3.0-8.0), followed by green oxidation to MnOx, pH 6.0 was identified as the optimal immobilization pH based on photocatalytic performance under identical experimental conditions (initial MB concentration: 10 ppm; pH: 7.0; solid-to-liquid ratio: 1:1, light exposure time: 2 hours). Under these conditions, the MnOx/BN nanocomposite achieved a removal efficiency of 94.5%. Furthermore, 52.3% of the MB solution was degraded within the first 5 minutes, indicating a rapid initial reaction rate. Moreover, the composite retained stable performance under varying pH and temperature conditions, indicating its suitability for real-world wastewater treatment applications. The use of *Stevia rebaudiana* extract as a natural reducing agent not only reduced environmental impact but

---

[1]Corresponding author

also offered a cost-effective synthesis alternative. These findings suggest that MnOx/BN nanocomposites have strong potential for scaling up and application in industrial wastewater treatment systems.

Keywords: biphasic nanostructures, metal oxide, nanocomposite, methylene blue, photocatalysis

Removal of Dyestuff from Aqueous Solutions using Magnetic Cerium Particles

Sadiye KARATAS[1] , Nagihan Karaaslan AYHAN[1,2]

[1]Department of Strategic Raw Materials and Advanced Technology Applications, Graduate Education Institute,
Munzur University, Tunceli, Türkiye.
[2]Department of Chemistry and Chemical Processing Technologies, Tunceli Vocational School,
Munzur University, Tunceli, Türkiye
[1]karatassdy@gmail.com, [2]nkaraaslan@munzur.edu.tr
[1](ORCID: 0009-0007-9104-4680), [2](ORCID: 0000-0001-9083-9149)

Abstract

Dyes used for coloring purposes in various industries, such as textiles, paper, paint, pharmaceutical, plastic, and automotive, are released into the environment with industrial wastewater and cause significant environmental pollution. Inorganic and organic pollutants released into the environment through wastewater are carcinogenic, toxic, and pose a threat to both living and non-living life. Wastewater must be treated to prevent environmental pollution and maintain ecological balance. Adsorption is generally the preferred method for wastewater treatment [1-2]. In this method, natural adsorbents such as chitosan, alginate, and zeolite have been preferred as adsorbents in recent years because they are non-toxic, biodegradable, environmentally friendly, and reusable [3-6]. Alginate, a natural adsorbent, is a salt of alginic acid, obtained from algae, and reacts with multivalent cations to form polymeric beads. These polymeric beads are used to remove various pollutants from wastewater. Studies on the removal of dye, fluoride and phosphate from wastewater with different adsorbent materials prepared using alginate have been reported in the literature [7-11].

This study investigated the removal of malachite green dye from aqueous solutions using magnetic cerium particles and adsorption. Magnetic cerium particles were obtained using an ionic cross-linking method. Previously synthesized iron particles were used for this purpose [4]. The adsorbent material was obtained by ionic cross-linking with cerium, a rare earth element, using an alginate solution containing iron particles. Subsequently, parameters such as pH, time, and adsorbent amount, which would affect the experimental procedure in this study, were optimized. Adsorption isotherm and kinetic studies were conducted under optimum conditions. The results demonstrated that magnetic cerium particles are effective in removing malachite green dye and can be used for dye removal in wastewater.

Keywords: dye, cerium, magnetic, optimization

Acknowledgment: This study was supported by The Scientific Research Projects Coordination Unit of Munzur University (Grant numbers: YLMUB023-12).

References

[1] Homagai, P.L., Poudel, R., Poudel, S., Bhattarai, A., 2022. Adsorption and removal of crystal violet dye from aqueous solution by modified rice husk. Heliyon, 8:e09261.
[2] Tewari, K., Singhal, G., Arya, R.K., 2018. Adsorption removal of malachite green dye from aqueous solution. Reviews In Chemical Engineering, 34:427-453.
[3] Li, C.J., Zhang, Y.J., Chen, H., He, P.Y., Zhang, Y., Meng, Q., 2021. Synthesis of fly ash cenospheres-based hollow ABW zeolite for dye removal via the coupling of adsorption and photocatalysis. Advanced Powder Technology, 32:3436-3446.
[4] Ayhan, N.K., 2024. Lanthanum-based magnetic biopolymers for brilliant green removal from aqueous solutions. Environmental Science and Pollution Research, 31:47714-47726.
[5] Zhao, Y.T., Li, B.G., 2022. Preparation and superstrong adsorption of a novel La(III)-crosslinked alginate/modified diatomite macroparticle composite for anionic dyes removal from aqueous solutions. Gels, 8:810.
[6] Akha, N.Z., Salehi, S., Anbia, M., 2022. Removal of arsenic by metal organic framework/chitosan/carbon nanocomposites: Modeling, optimization, and adsorption studies. International Journal of Biological Macromolecule, 208:794-808.
[7] Kosari, M., Sepehrian, H., 2017. Fluoride ions removal using yttrium alginate biocomposite from an aqueous solution. International Journal of Engineering, 30:1-6.

---

[1] Corresponding author

[8] Feng, L.H., Zhang, Q., Ji, F.Y., Jiang, L., Liu, C.C., Shen, Q.S., Liu, Q., 2022. Phosphate removal performances of layered double hydroxides (LDH) embedded polyvinyl alcohol/lanthanum alginate hydrogels. Chemical Engineering Journal, 430:132754.

[9] Seker, S., Ayhan, N.K., 2023. Adsorption potential of neodymium/alginate beads for removal of Congo red and Brilliant blue G from aqueous solution. International Journal of Environmental Science and Technology, 20:7293-7304.

[10] Li, B.G., Yin, H.Y., 2020. Superior adsorption property of a novel green biosorbent yttrium/alginate gel beads for dyes from aqueous solution. Journal of Polymers and the Environment, 28:2137-2148.

[11] Li, B.G., Chen, C., 2022. Novel magnetic gel composite based on sodium alginate crosslinked by yttrium (III) as biosorbent for efficient removal of direct dyes from aqueous solution. Journal of Dispersion Science and Technology, 43:2142-2155.

Chemical Characterization of Lignocellulosic Biomass for Sustainable Biofuel Production

Gizem ÖZER[1], Neslihan DURANAY[2], Şeyda TAŞAR[3]

[1,2,3] Chemical Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[1]9314gizem@gmail.com, [2] nduranay@firat.edu.tr, [3]sydtasar@firat.edu.tr
[1](ORCID: 0000-0003-3610-8454), [2](ORCID: 0000-0001-7259-1864), [3](ORCID: 0000-0003-3184-1542)

Abstract

The world's population is projected to reach 8.5 billion by 2030 and 9.7 billion by 2050 [1], which is accelerating the consumption of energy, food, fuel, and basic chemicals. This trend has intensified the search for new, alternative, and sustainable resources. Biomass, which has attracted global attention as a renewable carbon source, exists in various forms and is utilized to produce heat, electricity, fuels, and other value-added by-products [2]. It is generally classified as municipal solid and sewage waste, agricultural and forestry residues, and biological waste. Lignocellulosic biomass obtained from agricultural and forestry residues is the only renewable energy source containing carbon and has been identified as a suitable feedstock for biofuel production [2]. However, much of this lignocellulosic waste is either discarded or burned as low-quality fuel, leading to the loss of renewable resources and causing significant environmental pollution. Biomass sources are considered carbon-neutral because the CO_2 emitted during combustion is balanced by the CO_2 absorbed by plants through photosynthesis [3]. Therefore, renewable carbon-containing resources derived from agricultural and forestry waste can be effectively used in the production of biofuels and other biochemicals [2]. Moreover, utilizing waste biomass for the production of biofuels and biomaterials embodies a "waste-to-wealth" approach, enhancing profitability throughout the energy production process [4].

Lignocellulosic biomass possesses a complex and heterogeneous structure composed primarily of three biopolymers: cellulose, hemicellulose, and lignin, along with minor amounts of extractives and ash [5]. Cellulose, a linear homopolysaccharide consisting of β-(1→4)-linked D-glucose units, forms crystalline microfibrils that provide mechanical strength and structural stability to plant cell walls. Hemicellulose is an amorphous heteropolysaccharide composed of various monosaccharides such as xylose, mannose, galactose, and arabinose, which act as a matrix between cellulose fibrils and lignin, contributing to flexibility and water retention. Lignin, a complex aromatic polymer rich in phenylpropanoid units, fills the spaces between cellulose and hemicellulose, imparting hydrophobicity, rigidity, and resistance to microbial degradation. This intricate lignocellulosic architecture confers remarkable durability to biomass but also presents challenges for conversion into biofuels, necessitating effective pretreatment strategies [5,6]. The first step in producing bioproducts from lignocellulosic feedstocks involves fractionating these structural components through pretreatment processes, which can be categorized as chemical (e.g., acid or alkali hydrolysis, organosolv), physical (e.g., milling, steam explosion), or biological (e.g., enzymatic hydrolysis) [7,8].

In this study, four different lignocellulosic biomass sources—almond shells, corn stalks, walnut shells, and pine sawdust—were chemically characterized to determine their extractive matter, cellulose, hemicellulose, and lignin contents. Pine sawdust exhibited a high extractive content attributable to its resinous nature and a cellulose proportion of 44.178%, indicating strong potential for producing high-yield biofuels via pyrolysis or enzymatic hydrolysis. Almond shells were found to contain 53.157% hemicellulose and 17.021% lignin, offering enhanced thermal stability and superior combustion properties due to the synergistic effects of hemicellulose devolatilization and lignin char formation. Walnut shells demonstrated a balanced distribution of cellulose and lignin, which may provide versatility in both biochemical (fermentation) and thermochemical (gasification, pyrolysis) conversion routes. Corn stalks, with relatively lower lignin content, could facilitate easier enzymatic saccharification, making them favorable for bioethanol production. These findings highlight the importance of compositional analysis in selecting feedstocks for targeted bioenergy pathways, as variations in cellulose crystallinity, hemicellulose branching, and lignin cross-linking directly impact conversion efficiency, product selectivity, and overall process sustainability [1,4].

Keywords: lignocellulosic biomass, sustainable energy, biofuel, biomass waste, chemical analysis

References

[1] Meneses, D. G., Vasquez, G. M., Baudrit, J. R., Roj, M., Castillo, J., & Araya, L. C. (2022). Pretreatment methods of lignocellulosic wastes into value-added products: Recent advances and possibilities. Biomass Conversion and Biorefinery, 12(2), 547–564. https://doi.org/10.1007/s13399-020-00722-0

---

[1] Corresponding author

[2] Yogalakshmi, K. N., Poornima, D. T., Sivashanmugam, P., Kavitha, S., Yukesh, K. R., Sunita, V., Adishkumar, S., Kumar, G., & Rajesh, B. J. (2022). Lignocellulosic biomass-based pyrolysis: A comprehensive review. Chemosphere, 286, 131824. https://doi.org/10.1016/j.chemosphere.2021.131824

[3] Gonzalez, P. I., & Rong, B. G. (2019). A review of the current state of biofuels production from lignocellulosic biomass using thermochemical conversion routes. Chinese Journal of Chemical Engineering, 27(7), 1523–1535. https://doi.org/10.1016/j.cjche.2018.09.018

[4] Chen, Z., Chen, L., Khoo, K. S., Gupta, V. K., Sharma, M., Show, P. L., & Yap, P. S. (2023). Exploitation of lignocellulosic-based biomass biorefinery: A critical review of renewable bioresource, sustainability and economic views. Biotechnology Advances, 69, 108265. https://doi.org/10.1016/j.biotechadv.2023.108265

[5] Ceylan, Z., Taşar, Ş., Kaya, F., & Özer, A. (2020). Farklı biyokütle atıklarının alkali ön işlem etkinliklerinin incelenmesi. Düzce Üniversitesi Bilim ve Teknoloji Dergisi, 8(4), 2296–2312. https://doi.org/10.29130/dubited.787863

[6] Ceylan, Z., Taşar, Ş., Kaya, F., & Özer, A. (2020). Kayısı çekirdeği kabuğu ve çay atığından makromoleküllerin izolasyon verimi üzerine alkali ön işlem parametrelerinin etkisi. Erzincan Üniversitesi Fen Bilimleri Enstitüsü Dergisi, 13(3), 1004–1015. https://doi.org/10.18185/erzifbed.769703

[7] Taşar, Ş., & Özer, A. (2022). A comparative study of hemicellulose isolation with hot water, alkaline, and delignification methods from tea leaf brewing waste. Biomass Conversion and Biorefinery, 12(7), 2501–2514. https://doi.org/10.1007/s13399-020-00752-8

[8] Taşar, Ş., & Özer, A. (2021). Synthesis and characterization of hemicellulose-based polymeric gel film from tea leaf brewing waste. Chemical Industry and Chemical Engineering Quarterly, 27(3), 265–277. https://doi.org/10.2298/CICEQ200810045T

Green Synthesis of Silver Nanoparticles from Walnut Shell Extract and Their Comparative Performance in PLA/Epoxy and PLA/PEG Biocomposites

Buket ERZEN[1], Mukaddes KARATAŞ[2], Ercan AYDOĞMUŞ[3], Ramazan ORHAN[4]

[1,2,3,4]Department of Chemical Engineering, Faculty of Engineering, Fırat University, 23119, Elazığ, Türkiye.
[1]bcetintas@firat.edu.tr, [2]mkozturk@firat.edu.tr, [3]ercanaydogmus@firat.edu.tr, [4]rorhan@firat.edu.tr
[1](ORCID: 0000-0001-5098-7171), [2](ORCID: 0000-0001-5803-6821), [3](ORCID: 0000-0002-1643-2487), [4](ORCID: 0000-0003-2287-4238)

Abstract

In recent years, environmentally friendly and sustainable production approaches have become increasingly important in chemical and materials engineering, as well as other engineering fields. The efficient use of natural resources, the recycling of waste, and the development of biodegradable materials are among the primary objectives [1]. Agricultural waste, in particular, is considered an important resource due to its richness and abundance of organic compounds, and must be converted into added value. Innovative methods must be developed to process these wastes without harming the environment. The development of nanotechnology has made the use of biogenic extracts obtained from agricultural waste an effective approach for producing environmentally friendly, economical, and low-toxic nanoparticles [2]. Silver nanoparticles (AgNPs) have a wide range of applications in various fields, including biomedicine and environmental technologies, due to their antibacterial, antioxidant, and electronic properties [3]. A common strategy is to reinforce AgNPs in biodegradable polymer matrices to improve stability and ease of use. Biodegradable polymers such as polylactic acid (PLA) have gained prominence in recent years due to their environmentally friendly structures and good mechanical properties. However, their brittleness and limited electrical properties can be improved using various additives [4]. Hybrid systems formed with polymers such as epoxy and polyethylene glycol (PEG) have the potential to enhance mechanical strength and functionality [5]. The homogeneous distribution of nanoparticles within the polymer matrix is critical for the performance of composites. Improved dispersion provides significant enhancements to mechanical strength, thermal stability, and electrical properties [6]. Significant emphasis has therefore been placed on dispersion techniques in the synthesis and composite manufacturing processes. This approach offers flexibility in material design and enables a wide variety of applications. It has also laid the groundwork for the integration of sustainable biocomposites into industrial processes. Furthermore, the aim is to minimize environmental impact.

This study aims to produce AgNPs using a green synthesis method involving walnut shell extract, utilizing the abundant waste product of walnut shells. A comparative performance analysis will be conducted by adding these nanoparticles to PLA/epoxy and PLA/PEG hybrid polymer systems at different ratios. The walnut shell provides a high level of reducing capacity and nanoparticle stability thanks to its rich content of phenolic compounds and tannins. The walnut shell extract was prepared in distilled water at specific ratios, mixed with an $AgNO_3$ solution, and allowed to react on a magnetic stirrer at room temperature. The phenolic compounds reduced the Ag^+ ions and also stabilized the nanoparticles as a natural capping agent. The AgNPs obtained after the reaction were then centrifuged and purified. Synthesis was carried out under controlled temperature and pH conditions to ensure reproducibility and homogeneity [7]. The resulting AgNPs were then integrated into PLA/epoxy and PLA/PEG systems at various ratios. Controlling the size and morphology of the nanoparticles and the synthesis parameters resulted in narrowly distributed, stable particles. Furthermore, the dispersion techniques employed in producing the composites aimed to ensure a balanced, homogeneous distribution of the AgNPs within the polymer matrix. This is critical for achieving significant improvements in the mechanical, electrical, and thermal properties of the composites.

Comprehensive analyses were conducted to evaluate the mechanical properties, density, Shore A hardness, thermal conductivity, thermal stability, dielectric constant, and microstructure of the developed biocomposites. Advanced techniques such as FTIR, XRD, SEM, and optical microscopy were employed in the characterization process. The analyses revealed an increase in Shore hardness of up to 10%, as well as a significant improvement in the dielectric constant, both of which increased with nanoparticle content. Bulk density decreased slightly, which was associated with micro-pore formation. Microscope images showed that a low nanoparticle content led to homogeneous distribution, whereas a higher content increased agglomeration tendencies, particularly in the PLA/epoxy system. Adding PEG improved the distribution of nanoparticles in the PLA/PEG system, reducing porosity and preserving structural integrity. Thermal analysis results showed that adding AgNPs had a positive effect on the thermal stability of the composites, thus enhancing their durability in high-temperature applications. These improvements in dielectric performance suggest that these biocomposites could be used in electrical insulation and sensor technologies.

Although there are various studies in the literature on synthesizing AgNPs using plant waste extracts as reducing and capping agents, and incorporating these nanoparticles into PLA-based composites, most have only examined a single polymer system [8] and have not conducted comparative analyses of their dielectric, mechanical, and microstructural properties. Furthermore, information on the optimal

---

[1] Corresponding author

addition ratios and uniform distribution of AgNPs in biodegradable matrices is lacking [9]. This study addresses these issues by comprehensively comparing AgNPs synthesized using walnut shell extract in two different polymer systems. The study also makes a significant contribution to the principles of the circular economy and industrial symbiosis by converting waste into valuable nanomaterials. This approach is a pioneering example of current research into developing sustainable production models.

The developed biocomposites have a wide range of applications in the biomedical field, including wound dressings, medical device coatings, active food packaging (to extend shelf life), low-voltage electrical insulation, flexible sensor technologies, and protective surface coatings [10]. The results show that adding 0.5 wt.% AgNPs provide an optimal balance of mechanical, electrical, and microstructural properties. However, dispersion homogeneity deteriorated at higher nanoparticle content. These findings are important for designing and producing biodegradable composites on an industrial scale. This study makes significant scientific and environmental contributions to sustainable material production and waste management. Furthermore, comparing the performance of AgNPs in different polymer systems offers new insights into biocomposite design. Future studies are recommended to optimize synthesis parameters and expand application areas.

Keywords: green synthesis, silver nanoparticles, polylactic acid, biocomposite, walnut shell extract, characterization, sustainable materials.

References

[1] Kim, M. S., Chang, H., Zheng, L., Yan, Q., Pfleger, B. F., Klier, J., Nelson, K., Majumder, E. L.W., & Huber, G. W. (2023). A review of biodegradable plastics: Chemistry, applications, properties, and future research needs. Chemical Reviews, 123(16), 9915–9939. https://doi.org/10.1021/acs.chemrev.2c00876

[2] Baraketi, S., & Khwaldia, K. (2024). Nanoparticles from agri-food by-products: Green technology synthesis and application in food packaging. Current Opinion in Green and Sustainable Chemistry, 49, 100953. https://doi.org/10.1016/j.cogsc.2024.100953

[3] Burdușel, A.-C., Gherasim, O., Grumezescu, A. M., Mogoantă, L., Ficai, A., & Andronescu, E. (2018). Biomedical applications of silver nanoparticles: An up-to-date overview. Nanomaterials, 8(9), 681. https://doi.org/10.3390/nano8090681

[4] Aleksanyan, K. V., Smykovskaya, R. S., Samoilova, N. A., Novikov, V. A., Shakhov, A. M., Aybush, A. V., Kuznetsova, O. P., Lomakin, S. M., & Ryzhmanova, Y. V. (2024). Development of Poly(lactic acid)-Based Biocomposites with Silver Nanoparticles and Investigation of Their Characteristics. Polymers, 16(19), 2758. https://doi.org/10.3390/polym16192758

[5] Wong, T. L., Ma, K., & Abeykoon, C. (2024). Enhancing the thermal performance of polyethylene glycol phase change material with carbon-based fillers. International Journal of Heat and Mass Transfer, 220, 124919. https://doi.org/10.1016/j.ijheatmasstransfer.2023.124919

[6] Rahman, M. M., Khan, K. H., Parvez, M. M. H., Irizarry, N., & Uddin, M. N. (2025). Polymer nanocomposites with optimized nanoparticle dispersion and enhanced functionalities for industrial applications. Processes, 13(4), 994. https://doi.org/10.3390/pr13040994

[7] Restrepo, C. V., & Villa, C. C. (2021). Synthesis of silver nanoparticles, effect of capping agents, and size and shape dependency: A review. Environmental Nanotechnology, Monitoring & Management, 15, 100428. https://doi.org/10.1016/j.enmm.2020.100428

[8] Bioplastics, G. Second and Third Generation Bioplastics.

[9] Harun-Ur-Rashid, M., Foyez, T., Krishna, S. B. N., Poda, S., & Imran, A. B. (2025). Recent advances of silver nanoparticle-based polymer nanocomposites for biomedical applications. RSC Advances, 15(11), 8480–8505. https://doi.org/10.1039/D4RA10572K

[10] Malik, K., Kazmi, A., Sultana, T., Raja, N. I., Bibi, Y., Abbas, M., ... & Bashir, M. N. (2025). A mechanistic overview on green assisted formulation of nanocomposites and their multifunctional role in biomedical applications. Heliyon, 11(3), e13687. https://doi.org/10.1016/j.heliyon.2025.e13687

Faunistic Contribution to Turkish Cicadellidae: First Record of Frutioidia (Frutioidia) bisignata (Mulsant & Rey, 1855) in Bingöl

Ceyhan SÖNMEZ[1], İnanç ÖZGEN[2]

[1,2] Firat University, Bioengineering Department, Elazığ, Turkey
[1]csonmez@firat.edu.tr , [2]inancozgen@gmail.com
(ORCID: 0000-0001-5894-2445), [2](ORCID: 0000-0003-1742-9324)

Abstract
This study reports the first faunistic record of *Frutioidia (Frutioidia) bisignata* (Mulsant & Rey, 1855) in Bingöl province, Eastern Turkey. A total of 88 specimens (55 females and 33 males) were collected in August 2025 from Crataegus monogyna using the Japanese umbrella method. The species, previously recorded in various regions of Turkey, is known to inhabit Rosaceae plants but has not been confirmed as a vector of plant pathogens. The new locality extends the known distribution of F. bisignata and highlights the need for further ecological and phytopathological research in Eastern Anatolia.

Keywords: *Frutioidia bisignata*, Cicadellidae, *Crataegus monogyna*, Bingöl province, Leafhopper, Hemiptera, Faunistic study, First record, Eastern Anatolia

1. Introduction

The family Cicadellidae (leafhoppers) includes numerous species of economic importance due to their ability to cause direct feeding damage and, more importantly, their role as vectors of plant pathogens such as viruses and phytoplasmas. Although many Cicadellidae species have been recorded in Turkey, the faunistic diversity of the eastern regions, including Bingöl province, remains underexplored.

Frutioidia (Frutioidia) bisignata (Mulsant & Rey, 1855) is a Palearctic species with a wide geographical distribution, including several countries across Europe and Western Asia (Dlabola, 1981; Lodos & Kalkandelen, 1984). In Turkey, the species has previously been reported from Adana, İzmir, Isparta, Giresun, and several other provinces (Bozbuğa & Elekçioğlu, 2008). It is known to inhabit grassy areas, shrubs, and orchards and is typically associated with members of the Rosaceae family. Documented host plants include *Crataegus* sp., *Malus* sp., *Prunus spinosa*, and *Prunus amygdalus* (Anonymous, 2025).

The species has also been recorded among leafhopper fauna associated with cherry trees in the Eastern Mediterranean Region (Kaya & Başpınar, 2020). However, despite its widespread presence, there is currently no evidence of *F. bisignata* acting as a phytoplasma or virus vector. A survey conducted in Lebanon, for instance, reported the species in high numbers within apricot orchards but noted no plant damage or vector activity (Anonymous, 2012).

This study documents the first faunistic record of *Frutioidia (Frutioidia) bisignata* from Bingöl province. The record contributes to our understanding of the distribution range of this species in Turkey and provides valuable baseline data for future ecological and phytopathological assessments in the region.

2. Material and Methods

Specimens of *Frutioidia (Frutioidia) bisignata* (Mulsant & Rey, 1855) were collected during a faunistic survey conducted in August 2025 within the province of Bingöl, Turkey. Individuals were sampled in the evening hours from natural populations of *Crataegus* sp. by employing the Japanese umbrella shaking method. The dislodged specimens were subsequently collected using an aspirator.

In the laboratory, the specimens were examined under a dissection microscope, and the necessary dissection procedures were performed to expose diagnostic morphological characters. High-resolution photographic documentation was prepared and archived digitally. The identification of the species was confirmed as *Frutioidia (Frutioidia) bisignata* by taxonomic specialist Dr. Francesco Poggi.

3. Results

Frutioidia (Frutloidla) bisignata (Mulsant et Rey, 1855) (Figure 1).

---

[1] Corresponding author

Material examined: Bingöl, Center, Çavuşlar, 19.08.2025, 55 ♀, 33♂, **Totally:** 88 exc.
Distribution in the World: Austria, Bulgaria, Cyprus, France, Greece (Euboea), Iran, Israel, Italy (also Sardinia), Jordan, Portugal, Spain, Switzerland, Tunisia, Turkey, Russia, Serbia , Iran (Dlabola, 1981; Lodos and Kalkandelen, 1984; Bozbuğa and Elekçioğlu, 2008).
Distribution in Turkey: Adana, Çankırı (Ilgaz) Giresun, Bitlis, Isparta, İzmir, Nevşehir, Karabük Trabzon, Ordu.
Biological note: Specimens were collected in late August on *Crataegus monogyna*

Figure 1. The habitus of *Frutioidia (Frutloidla) bisignata* (Mulsant et Rey, 1855) (Figure 1).

4. Discussions

During a faunistic survey conducted on 19 August 2025 in Çavuşlar, Bingöl (Eastern Turkey), a total of 88 specimens of *Frutioidia (Frutioidia) bisignata* (Mulsant & Rey, 1855) were collected from *Crataegus monogyna* plants. The sample comprised 55 females and 33 males. This record represents the first documentation of the species from Bingöl province and, more broadly, one of the few faunistic reports from the Eastern Anatolia Region.

Frutioidia bisignata has previously been recorded in various parts of Turkey, including Adana, İzmir, Isparta, Karabük, Giresun, and Nevşehir, among others (Lodos & Kalkandelen, 1984; Bozbuğa & Elekçioğlu, 2008). However, the species' presence in Bingöl a high-altitude, continental climate region indicates a potentially broader ecological tolerance and distribution range than previously assumed.

The specimens in this study were collected in the evening hours, using the Japanese umbrella method, a widely accepted and efficient technique for capturing arboreal Hemiptera. Their high numbers on *Crataegus monogyna* also reinforce previous records that associate this species with Rosaceae hosts (Anonymous, 2025).

Although *F. bisignata* has been found in economically significant crops such as cherry (Kaya & Başpınar, 2020) and olive (Bozbuğa & Elekçioğlu, 2008), there is no existing evidence that this species acts as a phytoplasma or virus vector. In a survey conducted in Lebanon, F. bisignata was recorded in large numbers within apricot orchards, yet researchers observed no plant damage or pathogen transmission, suggesting the species may not play a role in disease dynamics (Anonymous, 2012).

However, given its abundance in certain cultivated crops and ornamental plants, the vector potential of *F. bisignata* should not be entirely ruled out. Future studies incorporating molecular diagnostics (PCR/qPCR) and pathogen transmission tests are recommended to assess whether this species harbors or transmits phytopathogenic organisms under certain environmental or host conditions.

5. Conclusions

The confirmation of *Frutioidia (Frutioidia) bisignata* from Bingöl expands the known distribution of this Palearctic species within Turkey and contributes to the faunistic database of the Eastern Anatolia Region. While its ecological role currently appears neutral, ongoing monitoring and pathogen screening are essential, especially in the context of expanding agricultural production and climate-related shifts in vector-host dynamics.

Acknowledgments

The authors would like to express their sincere gratitude to Dr. Francesco Poggi for his valuable assistance in the identification of *Frutioidia (Frutioidia) bisignata* specimens.

6. References

[1] Anonymous, 2012. Pest Survey of Stone Fruit Crops in Lebanon (2011-2012). 118 p.

[2] Anonymous, 2025. Fruticidia bisignata(Mulsant & Rey, 1855) on *Crataegus*, etc. https://bladmineerders.nl/parasites/animalia/arthropoda/insecta/hemiptera/cicadomorpha/membracoidea/cicadellidae/typhlocybinae/erythroneurini/fruticidia/fruticidia-bisignata/?utm_source=chatgpt.com. Date: 29.08.2025.

[3] Kaya, K. and H. Başpınar, 2020. Determination of Species of Cicadellidae (Hemiptera) Family in Sweet CherryGrowing Areas of Eastern Mediterranean Region. Turkish Journal of Agriculture - Food Science and Technology, 8(7): 1502-1507.

[4] Bozbuğa, R. and N. Z. Elekçioğlu, 2008. Pests And Natural Enemies Determined In Olive Orchards in Turkey. Türk Bilimsel Derlemeler Dergisi 1 (1): 87-97.

[5] Lodos, N. and A. Kalkandelen, 1984. Preliminary list of Auchenorrhyncha with notes on distribution and importance of species in Turkey. XV. Family-Cicadellidae : Typhlocybinae Erythroneurini (Part I). Türk. Bit. Kor. Derg. (1984), 8: 159-168.

Synthesis of 1-(4-methoxybenzoyl)-4-(naphthalen-1-yl) thiosemicarbazide Compound and Investigation of its Experimental and Theoretical Spectra

Esra TOK[1], Murat GENC[2]

1 Department of Chemistry and Chemical Processing Technologies, Vocational School of Technical Sciences, Adiyaman University,
2 Department of Chemistry, Faculty of Arts and Sciences, Adiyaman University, 02040, Adiyaman, Turkey
[1]ebuyukaslan@adiyaman.edu.tr, [2]mgenc23@gmail.com
[1](ORCID: 0000-0002-4211-5995), [2](ORCID: 0000-0003-1224-4128)

Abstract

Biologically, cancer is characterized by abnormal cells separating from the primary tissue, exhibiting uncontrolled proliferation, and spreading to different areas through metastasis. Inhibiting this uncontrolled cell proliferation is one of the primary targets of anticancer treatment strategies. This effect can be achieved, in particular, by the application of chemical agents that disrupt the DNA replication process and thereby inhibit cellular proliferation[1]. Thiosemicarbazides, on the other hand, are known to be a group of organic compounds that can exert effects on various mechanisms involved in tumor formation, according to recent scientific reports [2]. Thiosemicarbazides are organic ligands containing nitrogen and sulfur, with a structure of $–NH–C(=S)–NH_2$ or its derivatives. The anticancer activity of thiosemicarbazide derivatives has been confirmed in numerous experimental and theoretical studies; the mechanisms of this effect are closely related to the presence and properties of substituent groups in the molecule [3] Furthermore, thiocarbazide derivatives exhibit promising biological activities due to their antimicrobial, antitumor, antiviral, anti-HIV, insecticidal, antisklerotic, antioxidant, antiparasitic, and anti-inflammatory effects and syntheses [2,4,5]. Thiosemicarbazides have a flexible structure due to their delocalized charge. This also allows for a range of coordination modes that have a significant impact on both structural and biological aspects [6]. Thiosemicarbazide derivatives have the ability to form intermolecular hydrogen bonds due to the presence of N–H proton-donating groups[4]. In particular, the presence of electron-donating ($–OCH_3$, $–CH_3$) and electron-withdrawing ($–NO_2$, $–Cl$) substituents has significant defining characteristics on DNA interactions and cell permeability. Researchers have shown particular interest in the use of thiosemicarbazide-based compounds as potential drug candidates due to their ability to interact with biological targets and modulate specific cellular pathways. [8] Again, from a biological effects perspective, thiosemicarbazide complexes are known to be able to pass through the semipermeable membrane of cells and exert anticancer therapeutic effects, generally by inhibiting DNA synthesis and increasing oxidative stress [10]. Hybrid molecules obtained from the synthesis reaction of thiosemicarbazides with triazoles are considered promising agents in the design of anticancer, antimicrobial, and antiviral agents from a pharmaceutical perspective, as they increase biological activity due to the combination of their structural and electronic properties. [11] These interactions at the molecular level enable the optimization of pharmacokinetic and pharmacodynamic properties of drugs, such as bioavailability, selectivity, and therapeutic efficacy.

This study focuses on the compound 1-(4-methoxybenzoyl)-4-(naphthalen-1-yl), synthesized as a novel thiosemicarbazide derivative that will contribute to the literature. The aim is to contribute to establishing the biological activities of this new derivative as a basis for applications such as anticancer drug development and antiviral and antimicrobial agent design.

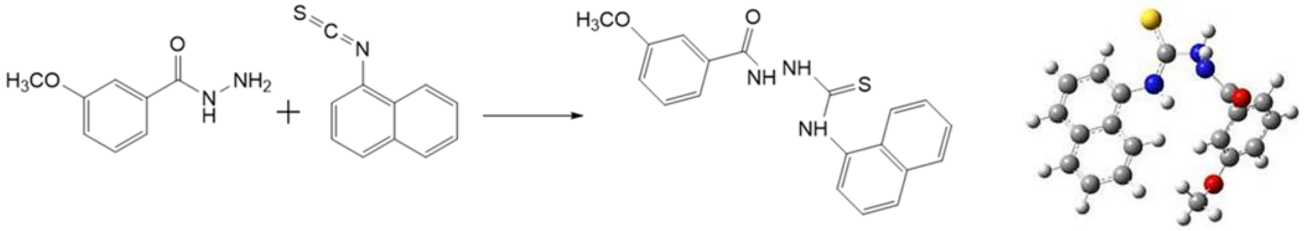


Figure 1: Synthesis Scheme of Thiosemicarbazide Derivative

The synthesized compound was evaluated using spectroscopic methods such as FT-IR, ^{1}H NMR, and ^{13}C NMR, as well as HOMO, LUMO analysis, and MEP maps. The FT-IR spectrum of the synthesized compound was measured using a PERKIN ELMER Spectrum 100 Spectrometer (Adıyaman University, Adıyaman), while the ^{1}H NMR and ^{13}C NMR spectra were measured using Nuclear Magnetic Resonance (NMR) Spectroscopy with a Bruker AscendTM 400 MHz Avance III HD (Inonu University, Malatya).

The HOMO-LUMO gap is defined as the energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). It is known as the energy difference between HOMO and LUMO and is

---

[1] Corresponding author

considered an important parameter that determines the chemical reactivity of molecules along with their electronic properties. HOMO represents the nucleophilic character of the molecule, which is its ability to donate electrons, while LUMO represents the electrophilic character, which is its tendency to accept electrons. A larger HOMO-LUMO gap indicates higher stability. HOMO–LUMO analysis is used as a specific determinant in many scientific research areas, such as stability and reactivity assessments, photovoltaic material development, molecular electronics, and drug design.
HOMO–LUMO analysis showed that 1-(4-methoxybenzoyl)-4-(naphthalen-1-yl) thiosemicarbazide has a suitable energy gap. This indicates an appropriate balance between stability and reactivity for biological interactions.

The MEP map (Molecular Electrostatic Potential Map) is a method that visualizes a molecule's electron density and, consequently, its positive or negative charge distribution in three dimensions. These maps are used to predict a molecule's reactivity, identify regions susceptible to nucleophilic or electrophilic attack, and understand weak interactions such as intermolecular hydrogen bonding, ion-dipole, and π-π interactions. They are also considered an important theoretical chemistry tool in drug design for identifying potential active regions that could bind to target proteins. For this purpose, nucleophilic or electrophilic attack-prone regions, weak interactions such as intermolecular hydrogen bonding, ion-dipole, and π-π interactions were defined by considering the MEP map of the compound 1-(4-methoxybenzoyl)-4-(naphthalen-1-yl) thiosemicarbazide.

MCF-7 (breast cancer cell line) cells are known as estrogen receptor-positive (ER+) cells. Aromatic and lipophilic structures generally provide an advantage in binding to receptors or enzymes in this cell line. The ligand–protein interaction map obtained from the molecular docking analysis of the 1-(4-methoxybenzoyl)-4-(naphthalen-1-yl) thiosemicarbazide compound on Mcf7 cancer cells (breast cancer cells) was also evaluated. In this context, it was observed that the compound 1-(4-methoxybenzoyl)-4-(naphthalen-1-yl) thiosemicarbazide may exhibit antiproliferative activity in MCF-7 cells.

Thiosemicarbazide derivatives are known to have pronounced cytotoxic effects on L1210 (leukemia cell line) cells, particularly by suppressing DNA synthesis and inhibiting cellular enzyme activities. For this purpose, the effects of the compound 1-(4-methoxybenzoyl)-4-(naphthalen-1-yl) thiosemicarbazide on L1210 (leukemia cells) were evaluated based on the ligand–protein interaction obtained from molecular docking analysis. The compound's ability to obtain a stable conformation in the binding region, along with the limited level of negative interactions, was seen to support the molecule's compatible binding with the target protein.

Characterization results confirmed the synthesis of the compound. This new thiosemicarbazide derivative demonstrated potential as a candidate for pharmacological applications in the investigation of biological activities.
All these computational methods provided valuable data on the structural, electronic, and pharmacological properties of the compound, serving as a basis for further in vitro and in vivo studies.

Keywords: Thiosemicarbazide, anticancer, NMR, FTIR

References

[1] Barbara Kaproń , Anita Płazińska , Wojciech Płaziński b, Tomasz Plech ,2022, Identification of the first-in-class dual inhibitors of human DNA topoisomerase IIα and indoleamine-2,3-dioxygenase 1 (IDO 1) with strong anticancer properties, J Enzyme Inhib Med Chem. 2022 Nov 8;38(1):192–202.

[2] Łucja Justyna Walczak-NowickaAleksandra Szopa , Monika Pitucha, Anna Şerefk, Anna Pachuta, Kamil Pawłowski, Monika Gawrońska-Grzywacz, Joanna Lachowicz and Mariola Herbet, 2024, Newly synthesized derivatives with a thiosemicarbazide group reduce the viability of cancer cell lines. Acute toxicity assessment in Zebrafish (Danio rerio) early life stages, Toxicology in VitroMarch, Vol 95, 105741

[3] Paweł Kozyra , Ewelina Humeniuk , Marta Arczewska , Grzegorz Adamczuk ,Mariusz Gagoś , Agnieszka Korga-Plewko , Monika Pitucha , 2025, Synthesis, in silico and in vitro studies and FTIR microspectroscopy of new thiosemicarbazide derivatives with potential antimelanoma activity, Bioorganic Chemistry, Volume 163

[4] Monika Pituch ve,Marcin Świątkowski ve, Ewelina Humeniuk ,Grzegorz Adamczuk ,Monika Drózd ve,Zbigniew Karczmarzyk,Elżbieta Kuśmierek ve,Krzysztof Strzelec ve,Anita Raducka ve,Waldemar Wysocki, Alina Olender fAnna Kozubg,Dorota Kowalczuk Ewa Poleszak , Agnieszka Czylkowska, 2024, Structure-activity relationship and cytotoxicity of the new thiosemicarbazide derivatives and their Cu(II) complexes against prostate and melanoma cancer cells, Archives of Biochemistry and Biophysics, Vol 755, 109955

[5] Prachi T. Acharya, Zeel A. Bhavsar, Divya J. Jethava, Dhaval B. Patel, Hitesh D. Patel, 2021, A review on development of bio-active thiosemicarbazide derivatives: Recent advances, Journal of Molecular Structure

[6] Volume 1226, Part A, 129268

[7] Shivendra K. Pandey , R. Chaurasia , Alok Shukla , Riya Kumari , Nishant Shekhar ,Arti Srivastava , A. Acharya , R.J. Butcher , M.K. Bharty , 2025, Exploring the anticancer activity of 1-(2-methyl-3-furoyl)-4-phenyl-3-thiosemicarbazide and its Mn(II) complex: Synthesis, spectral, crystal structures, and Hirshfeld surface analysis, Journal of Molecular Structure, ,Volume 1319, Part 1, 5 January 2025, 139426.

[8] Sinara Mônica Vitalino de Almeida 1 2, Elizabeth Almeida Lafayette 3, Lúcia Patrícia Bezerra Gomes da Silva 4, Cézar Augusto da Cruz Amorim 5, Tiago Bento de Oliveira 6, Ana Lucia Tasca Gois Ruiz 7, João Ernesto de Carvalho 8 9, Ricardo Olímpio de Moura 10, Eduardo Isidoro Carneiro Beltrão 11, Maria do Carmo Alves de Lima 12, Luiz Bezerra de Carvalho Júnior 13,2015, Synthesis, DNA Binding, and Antiproliferative Activity of Novel Acridine-Thiosemicarbazone Derivatives, Int J Mol Sci.;16(6):13023-42.

[9] Shivendra K. Pandey, R. ChaurasiaM. , Alok Şukla ,Riya Kumari ve,Nishant Shekhar ,Srivastava'nın Eseri,A. Acharya ,RJ Kasap ,K. Bharty, 2025, Exploring the synthesis, characterization, crystal structures, DFT calculation, hirshfeld surface analysis, and anticancer activity of Ni(II) complex of 1-(4-nitrobenzoyl)-4-phenyl-3-thiosemicarbazide, Journal of Molecular Structure, Volume 1321, Part 4, 140114

[10] Ram Nayan Gautam , Alok Shukla , Suryansh Chandra , Sundeep Kumar , A. Acharya ,Mamata Singh , R.J. Butcher , M.K. Bharty , 2025, Anticancer evaluation of Co(III) complex derived from 1-isonicotinoyl-4-(4-nitrophenyl)-3-thiosemicarbazide: Structural characterization,

[11] photophysical, and Hirshfeld studies Inorganic Chemistry Communications Volume 171, 113521)

[12] Vahideh Hadigheh Rezvan, 2024,Molecular structure, HOMO–LUMO, and NLO studies of some quinoxaline 1,4-dioxide derivatives: Computational (HF and DFT) analysis , Results in Chemistry, Volume 7, 101437

[13] Naveen , Ram Kumar Tittal, Vikas D. Ghule , Nikhil Kumar , Lokesh Kumar , Kashmiri Lal , Ashwani Kumar , 2020, Design, synthesis, biological activity, molecular docking and computational studies on novel 1,4-disubstituted-1,2,3-Triazole-Thiosemicarbazone hybrid molecules, Journal of Molecular Structure Volume 1209, 127951.

Thermochemical Valorization of Microalgal Biomass: Insights into Torrefaction and Pyrolysis Pathways for Sustainable Bioenergy Production (Mini- Review)

Gülşah YILDIZ[1], Şeyda TAŞAR[2], Elif KARDAŞ[3], Melek YILGIN[4]

[1,2,3,4] Chemical Engineering Department, Engineering Faculty, Firat University, Elazığ, TURKEY.
[1] gulsah093@hotmail.com, [2]sydtasar@firat.edu.tr; [3]elifkardas4@gmail.com; [4]myilgin@firat.edu.tr
[1](ORCID: 0009-0007-2706-963X), [2](ORCID: 0000-0003-3184-1542), [3](ORCID: 0000-0003-4726-0072); [3](ORCID: 0000-0002-4177-8025)

Abstract

Growing environmental concerns, rising global energy demand, and the rapid depletion of fossil fuels have made the shift toward renewable energy sources a global necessity [1, 2]. The limitations and environmental harms of conventional energy systems have accelerated the search for cleaner and more sustainable alternative clean energy biobased resource [2]. Among these, microalgae have attracted increasing attention as third-generation bioenergy feedstocks due to their exceptional biological and ecological characteristics [4]. With high photosynthetic efficiency, rapid biomass production, and the ability to grow on non-arable land using saline or wastewater instead of freshwater, microalgae contribute to energy generation without competing with food production [5]. Additionally, their ability to fix atmospheric carbon dioxide (CO_2) makes them a strategic resource for both renewable energy and climate change mitigation [6]

This brief review focuses on the role of microalgae in thermochemical conversion technologies, particularly torrefaction and pyrolysis processes [7, 8, 9]. Torrefaction, typically conducted in an inert atmosphere at temperatures between 200–300 °C, is known as a mild thermal pretreatment that enhances the fuel properties of biomass [10]. This process increases energy density, improves structural integrity, reduces moisture content, and enhances water resistance, making the biomass more suitable for subsequent energy conversion methods such as pyrolysis or gasification. In microalgae, torrefaction facilitates the breakdown of cellular structures, alters surface properties, and reduces the oxygen-to-carbon ratio, directly influencing pyrolytic behavior.[11, 12].

This mini-review was evaluated how torrefaction affects product yields (bio-oil, syngas, biochar), energy recovery, and emission profiles during the pyrolysis of microalgal biomass. Due to microalgae's higher protein and lipid contents and lower lignin levels compared to conventional lignocellulosic biomass (such as wood, straw, or agricultural residues), microalgae follow different thermal decomposition pathways. These differences significantly influence volatile release, char formation, and gas composition.

In this study aims to provide a comprehensive overview of the thermochemical valorization of microalgae by synthesizing recent findings in the literature. The insights offered can help guide experimental research, inform process optimization strategies, and support the development of environmentally friendly, scalable bioenergy technologies.

Keywords: microalgae, biomass, torrefaction, thermochemical conversion, renewable energy

References

[1] Holechek, J. L., Geli, H. M., Sawalhah, M. N., & Valdez, R. (2022). A global assessment: can renewable energy replace fossil fuels by 2050?. *Sustainability*, *14*(8), 4792.
[2] Singh, S. (2021). Energy crisis and climate change: Global concerns and their solutions. Energy: crises, challenges and solutions, 1-17.
[3] Lee, J. Y., Lee, S. E., & Lee, D. W. (2022). Current status and future prospects of biological routes to bio-based products using raw materials, wastes, and residues as renewable resources. Critical Reviews in Environmental Science and Technology, 52(14), 2453-2509.
[4] Powar, R. S., Yadav, A. S., Ramakrishna, C. S., Patel, S., Mohan, M., Sakharwade, S. G., ... & Sharma, A. (2022). Algae: A potential feedstock for third generation biofuel. Materials Today: Proceedings, 63, A27-A33.
[5] Omokaro, G., & Nafula, Z. S. (2023). Microalgae: Harnessing Environmental and Nature Benefits-A Comprehensive Review. American Journal of Agricultural Science, Engineering, and Technology, 7(3), 10-54536.
[6] Iglina, T., Iglin, P., & Pashchenko, D. (2022). Industrial CO2 capture by algae: a review and recent advances. Sustainability, 14(7), 3801.

---

[1] Corresponding author

[7] Mofijur, M., Hasan, M. M., Fattah, I. M. R., Huang, Y., & Shahriar, S. (2024). Thermochemical conversion of microalgae into biofuels. In Waste Valorization for Bioenergy and Bioproducts (pp. 315-333). Woodhead Publishing.

[8] Sutejo, G., Dewayanto, N., Suyono, E. A., & Budiman, A. (2022, December). Technology selection of microalgae thermochemical conversion to bio-crude oil. In *IOP Conference Series: Earth and Environmental Science* (Vol. 1105, No. 1, p. 012016). IOP Publishing.

[9] Rai, P., & Pandey, A. (2024). Chemical, biochemical, and thermochemical conversion of microalgal biomass into biofuel generation. In Microalgal Biomass for Bioenergy Applications (pp. 145-164). Woodhead Publishing.

[10] Khan, M., Uddin, S., & Razzak, S. A. (2025). Torrefaction of microalgal biomass for enhanced fuel properties and sustainability. Chemical Engineering Journal, 520, 166273.

[11] Zhang, C., Wang, M., Chen, W. H. H., Zhang, Y., Pétrissans, A., Pétrissans, M., & Ho, S. H. H. (2023). Superhydrophobic and superlipophilic biochar produced from microalga torrefaction and modification for upgrading fuel properties. *Biochar*, *5*(1), 18.

[12] Zhang, C., Fang, J., Zhan, Y., Wang, X., Chen, T., Hao, K., ... & Wang, Y. (2024). Life Cycle Assessment of Microalgal Carbon Fixation and Torrefaction for Carbon Neutralization: A State-of-the-Art Review. Green Energy and Fuel Research, 23-38.

Fabric Defect Detection Using Synthetic Defect Augmentation and Deep Learning

Zeynep SÖNMEZ[1] , Mert İNCİDELEN [2]

[1,2]Department of Artificial Intelligence and Data Engineering, Faculty of Engineering, Firat University, Elazig, Turkey.
[1]zeynepsonmezw@gmail.com, [2]mincidelen@firat.edu.tr
[1](ORCID: 0009-0007-0527-9126), [2](ORCID: 0009-0002-1975-8332)

Abstract

1. Introduction

A growing population and the accompanying rapid rise in consumption rates are necessitating significant changes in the global economy. One of the sectors where this change is most evident is the textile industry. This growing demand requires the adoption of high-volume production processes in this sector [1]. Maintaining high product quality alongside high-volume production is a critical factor in achieving competitive advantage today. Therefore, while increasing production capacity, quality control processes must also adapt to the increased speed and scale. Traditional quality control methods prove inadequate for high-volume production lines [2]. Defects are often overlooked during visual inspection [3]. Artificial intelligence-assisted solutions for defect detection in various sectors have the potential to offer more effective performance than traditional quality control systems, owing to their high accuracy [4]. Studies on artificial intelligence-based defect detection are widely reported in the literature within the textile industry [5–7] and other industrial domains [8–10]. In our study, synthetic defect generation was performed using a limited number of textile images, with a focus on defect detection in textile products.

2. Materials and Methods

In our study, the TILDA dataset [11], which is widely used in the literature for textile defect detection, was employed. From the plain fabric subset of the dataset, 100 images per class (defect-free, hole/tear, stain, and yarn defect) were selected, resulting in a total of 400 real images. In addition to these real images, the defect-free class was augmented using rotation, horizontal flipping, cropping, and translation to increase its sample size. Synthetic defects corresponding to the three defect classes (hole/tear, stain, and yarn defect) were generated on the augmented defect-free images. Synthetic defect images were generated using the OpenCV Python library by adding hole/tear, stain, and yarn defect patterns to 500 defect-free images, resulting in a balanced dataset with 500 images per class. Model training was performed using the ResNet-18 architecture, with 80% of the data allocated for training and 20% for testing. ResNet-18 is an 18-layer deep residual network widely used for image classification tasks [12]. The final layer of the model was configured to classify four classes. The model was evaluated using accuracy and macro-F1 score metrics.

3. Results and Discussion

The model developed in this study was evaluated in two stages. In the first stage, only the original dataset was used, and the model achieved an accuracy of 96.25% and a macro-F1 score of 0.963. This result indicates that the model trained on the original data achieved satisfactory performance. In the second stage, the incorporation of synthetic defect data into the training set led to a measurable improvement in model performance. At this stage, accuracy reached 98.04% and the macro-F1 score reached 0.981. Our findings demonstrate that synthetic defect generation enhances the model's ability to distinguish different defect types. It can be concluded that synthetically generated data serves as a valuable supplement for deep learning-based models, particularly when only a limited number of original images are available.

4. Conclusion

In this study, synthetic defects were generated on a textile dataset with limited defect images, and defect detection was conducted using a deep learning-based model. The findings revealed that the incorporation of synthetic data into the model significantly improved performance. These results indicate that synthetic data augmentation can provide an effective and scalable solution for reliable and rapid quality control, particularly in high-volume textile production lines. Future studies may further enhance system performance by incorporating a wider range of defect types, larger datasets, and more advanced deep learning architectures.

---

[1] Corresponding author

Acknowledgment

This study was carried out within the scope of the project numbered 1919B012428544, supported by the Scientific and Technological Research Council of Türkiye (TÜBİTAK) under the ‘2209-A Research Project Support Programme for Undergraduate Students.

Keywords: fabric defects, synthetic data, deep learning

5. References

[1] Sabeenian R.S, Paul E, Prakash C. “Fabric defect detection and classification using modified VGG network”. The Journal of The Textile Institute, 114(7), 1032-1040, 2023.
[2] Papageorgiou E.I, Theodosiou T, Margetis G, Dimitriou N, Charalampous P, Tzovaras D, Samakovlis I. “Short survey of artificial intelligent technologies for defect detection in manufacturing”. 2021 12th International Conference on Information, Intelligence, Systems & Applications (IISA), Chania, Greece, 1-7, 12–14 July 2021.
[3] Selamet F. Derin öğrenme yöntemleri ile metalik yüzeylerde kusur tespiti ve sınıflandırılması = Defect detection and classification on metallic surfaces using deep learning methods. MSc Thesis, Sakarya Üniversitesi, Sakarya, Türkiye, 2023.
[4] Ngan H.Y.T, Pang G.K.H, Yung N.H.C. “Automated fabric defect detection—A review”. Image and Vision Computing, 29(7), 442-458, 2011.
[5] Wei B, Hao K, Gao L, Tang X. “Detecting textile micro-defects: A novel and efficient method based on visual gain mechanism”. Information Sciences, 541, 60-74, 2020.
[6] Chang X, Gu C, Liang J, Xu X. “Fabric defect detection based on pattern template correction”. Mathematical Problems in Engineering, 2018(1), 3709821, 2018.
[7] Şeker A. “Evaluation of fabric defect detection based on transfer learning with pre-trained AlexNet”. 2018 International Conference on Artificial Intelligence and Data Processing (IDAP), Malatya, Türkiye, 1-4, 28–30 September 2018.
[8] Zhang D, Hao X, Wang D, Qin C, Zhao B, Liang L, Liu W. “An efficient lightweight convolutional neural network for industrial surface defect detection”. Artificial Intelligence Review, 56(9), 10651-10677, 2023.
[9] Xie L, Cen X, Lu H, Yin G, Yin M. “A hierarchical feature-logit-based knowledge distillation scheme for internal defect detection of magnetic tiles”. Advanced Engineering Informatics, 61, 102526, 2024.
[10] Shafi I, Mazahir A, Fatima A, Ashraf I. “Internal defects detection and classification in hollow cylindrical surfaces using single shot detection and MobileNet”. Measurement, 202, 111836, 2022.
[11] Computer Vision Group, Freiburg. “TILDA Textile Texture Database”. https://lmb.informatik.uni-freiburg.de/resources/datasets/tilda.en.html (18.07.2025).
[12] He K, Zhang X, Ren S, Sun J. “Deep residual learning for image recognition”. Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR), Las Vegas, Nevada, USA, 770-778, 27–30 June 2016.