RESUME

"Experience the greatest desires through the travel of wisdom."

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Skill sets- Catalysis; DFT study; Numerical Modelling study.

EDUCATION- PhD, Chemical Engineering- Indian Institute of Technology Roorkee, India.

Thesis Title-Synthesis and characterization of praseodymium and zirconium-based catalysts for dimethyl carbonate synthesis.

DATE OF Defense- 31st May 2024.

CGPA-7.8/10

MTech, Chemical Engineering- Dr. A.P.J. Abdul Kalam Technical University Lucknow, Harcourt Butler Technological Institute Kanpur, India.

Dissertation- A thesis on Reactive extraction of Acetic Acid.

Percentage- 69 %

BTech, Chemical Engineering- Chatrapati Sahu Ji Maharaj University, University Institute of Engineering & Technology Kanpur, India.

Project- Design of a distillation column.

CGPA- 7.6/10

12TH – School- Pinewood School, Saharanpur; Percentage: 81 %.

Subjects: Physics, Chemistry, Mathematics, English, Physical Education.

10th – School- Sophia Girls' High School, Saharanpur; Percentage: 84.4 %.

Subjects: English, Hindi, Mathematics, Science, Social Science.



Achievements and Awards

2007- 3rd Prize in I.T.C General Knowledge Quiz held at district level.

2007- Sportsman-ship spirit award at school level.

2012- Presented Essay for UN Chapter.

2013- Magazine editor for college TECHFEST.

2016- 1st Prize in National Level Conference held by TEQUIP-II funded by World Bank.

2018- 1st Prize in Quiz in IIT Roorkee based on Women's Rights.

2019- 2nd Prize in Essay Competition in IIT Roorkee based on Water Conservation by Dr. B.R. Ambedkar.

2019- 3rd Prize in Collage competition on Disaster Mitigation, IIT Roorkee.

2020- Outstanding performance in "Ideathon" Vision 2040, from the Office of Principal Scientific Adviser,

COLLABORATION

PhD - DFT and experimental studies with PhD colleague Pankaj Kumar.

Guiding a BTech Intern Akriti Singh in catalyst preparation.

MTech- Collaborated with Sarvesh Patel in studying reactive extraction of acetic acid as well as propionic acid.

Research Associateship- Guiding Project assistant Ms. Rakshitha for FISCHER-TROPSCH Process.

Collaborative work with Prof. Shubhi Gupta, IIT Dhanbad, on green fuel synthesis.

SUMMARY RESEARCH WORK

Research Associate- January 8, 2024- Present- Hands-on training on Aspen HYSYS for studying some aspects of modelling. High Pressure reactor for synthesis of green chemicals. Experiment on FISCHER-TROPSCH process.

PhD research Work, Indian Institute of Technology Roorkee, India. (Prof. Vimal Chandra Srivastava, Prof. Vimal Kumar)-2018- 2024- Training on packed bed reactor for synthesis of chemicals. Literature study on production of Dimethyl carbonate from methanol, under Project "Engineering aspects of methanol and conversion of methanol to dimethyl carbonate," Project No. SERB-1182-CHD. Research on production of Dimethyl carbonate using methanol and propylene carbonate.

MTech dissertation, Harcourt Butler technological Institute, India. (Prof. Ashwani Kumar Rathore) -(2015-2017)

Extraction of acetic acid via reactive extraction using set of diluents and reactants. Optimized the best diluent to be used with the extractant.

BTech Project-(2011-2015)- Design of distillation column.

Skills, Software, Training

- > Transesterification, Green fuel, green energy, Alternative fuel, Catalysis, High pressure reactor.
- ➤ Characterization techniques- XRD, XPS, SEM, FE-SEM, TEM, NH₃-TPD, CO₂-TPD, GC.
- > DFT-Quantum Espresso.
- > Aspen HYSYS.
- > One-week hands-on Training certification for Density functional theory of materials: nano particles, thin films, unit cells on Quantum Espresso, by Centre for Advanced computational Research, New Delhi.
- Hands-on Training on Aspen HYSYS certification.

SOCIAL ASPECTS

Volunteered for the **NGO**, **V Care**, where green plants are planted around Saharanpur region, India for the environmental sustainability.

Article in National Magazine

Article Published in Science Reporter titled, "Dynamic Future of the fuel cells: From Earth to Mars."

REFERENCES

(1). Prof. Vimal Chandra Srivastava-

vimalfch@iitr.ac.in, Dean International Relations,

Indian Institute of Technology Roorkee

(2). Prof. Dipteek Parmar

d_parmar@rediffmail.com, Professor, Head of Civil Engineering,

Harcourt Butler Technical University Kanpur

(3). Prof. Shubhi Gupta

shubhi@iitism.ac.in

Assistant Professor,

IIT Dhanbad.

PUBLICATION LIST

Papers Published (International) Journals.

- Dahiya, S.; Srivastava, V. C.; Kumar, V. (2022). Dimethyl carbonate synthesis via transesterification of propylene carbonate using a titanium-praseodymium-based catalyst. Energy & Fuels, 2022, 36(21), 13148-13158.
- Dahiya, S., Kumar, P., Srivastava, V. C., & Kumar, V. (2023). Production of dimethyl carbonate using a zirconium–praseodymium-based catalyst from methanol and propylene carbonate: An experimental and DFT Study. Industrial & Engineering Chemistry Research, 2023, 62(18), 6920-6931.
- Dahiya, S., Kumar, P., Srivastava, V. C., & Kumar, V. An experimental and kinetic study toward the production of dimethyl carbonate via transesterification using zirconium-embedded eucalyptus leaves ash (ZrO₂-E) as a catalyst: A green approach
- Dahiya S., Raghuvanshi S.S., Sharma U.C., Srivastava D., Rathore A., Acetic acid extraction from aqueous solution using tributyl phosphate in modified soyabean oil, 2018, Vol. 6, No., 6, 1197-1199.

Papers under review.

- An experimental and DFT approach for the production of dimethyl carbonate using eucalyptus ash integration in magnesium- praseodymium based catalyst: Towards sustainability.
- Studying the complex formation of zirconium in N, N Dimethyl formamide (DMF) [ZrO(OH)2.(DMF)] using DFT calculations for catalyst synthesis to produce dimethyl carbonate via transesterification.
- Catalytic transesterification using modified trimetallic combination Fe/Ce/Ti promoting high redox cycle of Fe(II)/Fe(III), Ce(III)/Ce(IV) and Ti(III)/Ti(IV) to produce green chemical dimethyl carbonate

Conferences

- Dahiya, S.; Srivastava, V. C.; Kumar, V. Production of zirconia-praseodymium based catalyst, Advances in Chemistry and Chemical Engineering (ACCE, 2021), Department of Chemical engineering, SVNIT, Surat, India, April 16-17, 2021. (BAGGED BEST PAPER AWARD)
 - Dahiya, S.; Srivastava, V. C.; Kumar, V. An investigation of engineering aspects of methanol during its reaction with carbon–dioxide using zirconium-praseodymium based catalysts in the production of dimethyl carbonate, International Chemical Engineering Conference 2021, Dr. B.R. Ambedkar National Institute of Technology, Jalandhar, September 16-19, 2021. (BAGGED BEST PAPER AWARD)
- Dahiya, S.; Srivastava, V. C.; Kumar, V. Production of dimethyl carbonate and propylene glycol via transesterification using novel catalysts. IKSAD Publications 2022; ISBN- 978-625-8423-98-3.7th IZCSR 2022, Gaziantep, Turkey, Jan 21-23, 2022.
- Dahiya, S.; Srivastava, V. C.; Kumar, V., CHEMTSF-2022. Production of dimethyl carbonate using eucalyptus ash integration in magnesium-praseodymium based catalyst, Department of Engineering, IIT Roorkee, Sept. 8-10, 2022.
- Dahiya S., COP26 Targets: Curbing the increased amount of carbon dioxide in the atmosphere: Utilization of carbon dioxide and ash by producing an oxygenated "Dimethyl carbonate," 5th Global Summit of GADRI, Japan.