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# Artificial Intelligence (AI) in Chemical Processes

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BACKGROUND SUMMARY 10 years of faculty teaching and over 30 years of technical leadership of industrial R & D experience in the chemical and petrochemical industries. Ph.D. in Chemical Engineering with expertise that include: - conceptual process design - pilot plant design and operations - waste remediation and minimization - product development - supercritical fluid technology - process safety - process simulation (Aspen, Hysys) - relief vent sizing - sustainability - microreactor technology

TECHNICAL ACCOMPLISHMENTS & COMPETENCIES: • Coordination of corporate and external institutions research and development programs. • Conceptual design, process simulation, economic evaluations and design for varieties of specialty chemical processes including development of a microreactor technology for production of hydrogen peroxide. • Developed technology for on-site production of both peracetic acid and hydrogen peroxide. • Worked on alternative technology to incineration to remove phosphine and cyanide • Worked on polymerization process in supercritical carbon dioxide to produce low molecular weight polymers with application in biodegradable products. • Supercritical fluid technology for use in both polymerization reactions and extraction of contaminants to produce products targeted to meet FDA/EPA requirements. • New method of synthesis for production of an agricultural chemical. Created a process for the recovery of acetic acid by-product which will generate $2 - 3MM annual savings. • Practical solution to prevent runaway polymerization of acrylic acid which significantly reduced safety hazards during transportation and storage.

SKILLS • Proven track record of leadership in interpersonal relationship to get work done efficiently with excellent research and analytical capability. • Strong ability to work across multiethnic environment and global technological collaboration across disciplines. • Transferable high level expertise in process engineering, project development, and innovative research from industrial setting to academia.

QUALIFICATIONS: Ph.D. Chemical Engineering, Lehigh University, 1989 M.S. Chemical Engineering, Lehigh University, 1986 B.Sc. Chemical Engineering, University of Ife, Nigeria, 1980

TEACHING EXPERIENCE: PRAIRIE VIEW A &M UNIVERSITY, Prairie View, TX , USA 2012 - Present

Assistant Professor, Department of Chemical Engineering 2018 - Present Adjunct Faculty Position, Department of Chemical Engineering 2012-2018 • Taught Chemical Process Safety CHEG 4103, Senior Design and Professionalism I CHEG 4473 , Senior Design and Professionalism II CHEG 4483, Process Design and Analysis CHEG 4043, Design of Process Engineering System CHEG 4183, Chemical Engineering Laboratory CHEG 1021(Summer, Bridge Program), Engineering Project Management GNEG 3061, Introduction to Petroleum Engineering GNEG 5193 & CHEG 4103; Heat, Mass, and Momentum Transport CHEG 3013, Introduction to Thermodynamics I & II CHEG 2043 & 3053, Unit Operations CHEG 3023, Chemical Process Safety CHEG 4103-P23, Introduction to Energy Systems, CHEG 3113and MITES Summer Program. • Developed curriculum for Chemical Process Safety CHEG 4103 course which was taught for the first time in PVAMU (Prairie View A & M University) at the spring semester 2013. • Developed curriculum for Engineering Project Management course, GNEG 3061 which was first introduced as a new course at PVAMU fall semester 2013. • Organized Aspen Training workshop for senior students, 2013, 2014, 2015, 2016 and 2017. • Supervised students attending NOBCChE Conferences. • Initiated the granting of the ICAS-Users-Educational-Version Software to the department. (ICAS is the Integrated Computer Aided System developed by Technical University of Denmark.) • Faculty Advisor to AIChE Student Chapter, PVAMU 2013 – present • Supervised Senior Design Projects 2012 – present • Served as mentor to the REU (Research Experience for Undergraduate) Program, Summer, 2017

LEHIGH UNIVERSITY, Bethlehem, PA, USA 1985 - 1989 Teaching Assistant in graduate and undergraduate courses in chemical engineering. UNIVERSITY OF PORT HARCOURT, Port Harcourt, Nigeria 1981 - 1984 Assistant Lecturer in undergraduate courses/instructions in chemical engineering. RIVERS STATE UNIV. OF SC. & TECH., Port Harcourt, Nigeria 1980 - 1981 National Youth Service (NYSC) instructor in undergraduate chemical engineering courses.

TECHNICAL EXPERIENCE: CHEMPROCESS TECHHNOLOGIES (CPT), LLC, League City, TX, USA 2010 – Present President and CEO: Consulting on Reactive Distillation, Waste Heat Recovery Technology, Energy Efficient Processes, Process Intensification, Process Synthesis and Design Co-PI on $1.1 million 2-year DOE funded research on Heat Integrated Reactive Distillation PI on $300K 1-year DOE Funded Grand Challenge FMC Project on Waste Heat Recovery Consultant to E3TEC Services on $120K 9-month DOE SBIR Project on Heat Enhancement Consultant to Safe Foods Corporation, Arkansas on Production of Peracetic Acid, Dec 2016

FMC CORPORATION, Princeton, NJ/Pasadena, TX, USA 1995- 2009 Associate Research Fellow, FMC Corporation, 2004 – 2009 Senior Research Engineering Associate FMC Corporation, 2001 – 2004 Research Engineering Associate, FMC Corporation, 1998 - 2001 Senior Research Engineer, FMC Corporation, 1995 - 1998 Led FMC's efforts in the DOE funded $1.5 million 5-year (2002 to 2007) project to develop (jointly with Stevens Institute) a novel microchannel reactor design for the production of hydrogen peroxide by the direct combination of hydrogen and oxygen with significance results. Developed mathematical models, conceptual design, economic analysis, and carried out steady state simulation using ASPEN Plus, Hysys and other simulators for varieties of specialty chemical processes. Developed and evaluated a proprietary technology for a hydrogen peroxide production process for use in the electronics and pulp & paper mills industries. Developed a supercritical extraction technique for the drying of a specialty battery solution product. Evaluated competitive technologies. Developed proprietary technology for peracetic acid processing and formulation.

ROHM AND HAAS COMPANY, Bristol, PA, USA 1989 - 1994 Research Engineer, Ag Chemical Process Research 1993 - 1994 Initiated and developed acetic acid recovery program and participated in a pilot plant operation of new agricultural products. Played a key role in team design effort to consolidate, upgrade and improve herbicides agricultural products plant of-the-future. Research Engineer, Process Technology Network 1992 - 1993 Coordinated and researched into waste remediation/handling technology. Participated in bringing new technology into the company. And evaluated competitive technologies for process improvements. Research Engineer, Fundamental Chemical Engineering Research 1989 - 1992 Developed supercritical fluid technology program in the areas of high pressure phase equilibria studies, polymerizations and purification/extraction of contaminants/residuals of polymer products.

SYNERGETSTIC ACTIVITIES Professional Affiliations: Fellow, American Institute of Chemical Engineers (AIChE); Fellow, Nigerian Society of Chemical Engineers (NSChE); Member, American Chemical Society (ACS); Member, National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE).

Committee Chair: Chair of MAC-AIChE Students Awards (1998- present); Chair Societal Impact Operating Council of AIChE (2006-07); Chair, MAC-AIChE (2000-2003), Chair, NSChE-USA Chapter (2002- Present); President, NOBCChE NY-NJ Chapter (2002-2009); Treasurer, NOBCChE NY-NJ Chapter (2009 - present)

Proposal Reviewer: Reviewed Proposals for DOE SBIR Program (2008); Reviewed Proposals for NSF (2011, 2012 and 2013), Reviewed Proposals for DOE Advanced Manufacturing Office Program, 2017

Journal Reviewer: Industrial & Engineering Chemistry Research Journal (2013)

Conferences: Chair, "Effective Mentoring for Students and Professionals in Chemical Engineering to Achieve Diversity in Workplace" session, AIChE's Annual 2001 Meeting, November 4-9, 2001 in Reno, Nevada; Co-Chair , "Process Improvement in Manufacturing" session, AIChE Spring 2002 Meeting, March 13, 2002 in New Orleans, LA; Co-Chair, "The Business Case for Sustainable Development" session ,AIChE Spring, April 25, 2007 in Houston, TX; Chair, "MAC Eminent Chemical Engineers Forum"

(2009-present);Chair, General Arrangement Committee (GAC) for the AIChE Centennial, Philadelphia, November 2008

COLLABORATORS AND OTHER AFFILIATIONS , USA

(i) Agblevor, F., Utah State University; Yusuf Adewuyi, NCA &T; Luke Achenie, Virginia Tech., Bruce Eldridge , UTexas at Austin; Aspi Kolah, Michigan State Univ. (MSU); Michael Harold, Univ. of Houston; Robert Ofoli, MSU; Rafiqul Gani, Technical Univ. of Denmark; Oluwafemi Taiwo, Obafemi Awolowo University, Ile-Ife, Nigeria; Irvin Osborne-Lee, Kazeem Olanrewaju & Michael Gyamerah, PVAMU, Prairie View. ii) Argonne National Laboratory : DOE Project on Heat Integrated Reactive Distillation.

HONORS AND AWARDS

• Elected Fellow AIChE (American Institute of Chemical Engineers), January 27, 2009 • Elected Fellow NSChE (Nigerian Society of Chemical Engineers), October 9, 2004 • Pioneer Award at MAC@25 AIChE, 2015 • The NOBCChE- Joseph N. Cannon Award for Excellence in Chemical Engineering 2014 • Nominated for Faculty Teaching Award, College of Engineering, PVAMU 2014 & 2015 • MAC-AIChE William Grimes Award for Excellence in Chemical Engineering 2012 • MAC-AIChE Black Achiever in Chemical Engineering 2008 • Featured in both the worldwide AIChE membership drive brochure and the AIChE Extra in the Chemical Engineering Progress (CEP) for his leadership contributions to AIChE, 2006. • NSChE (Nigeria Society of Chemical Engineers) Presidential Merit Award, 2002 and 2012 • MAC-AIChE Distinguished Service Award, 1999 • Distinguished High School SAT Mentor Award, NOBCChE Delaware Valley Section 1992

SERVICE TO THE SOCIETY, USA • Initiated and assisted in the collaboration between NOBCChE (National Organization for the Professional Advancement of Black Chemists and Chemical Engineers) and NSChE (Nigerian Society of Chemical Engineers) that led to a MOU (memorandum of understanding) , 2009 • Chairman, MAC-AIChE College Scholarship program from 1999 - present. Oversee the award and mentoring of more than 350 scholarships recipients to minority students with few Prairie View A & M University former students among the recipients. Sought corporate funding . • Reactivated the Janice Lumpkin Travel Award to AIChE Conference for minority Graduate students and professionals 2012 - present • Member Board of Directors of Community Capital Advisors (CCA), a resource institution based in Philadelphia, PA that is dedicated to social change and community economic development to alleviate poverty in distressed city communities, 2006 - present. • Served as a member and mentor (to some of the recipients) of the ACS Scholars Program for eight years (1999 - 2007) that awarded on the average 300 scholarships annually to underrepresented minorities. • Initiated and oversee the Bill Hills Memorial Scholarship to the outstanding African-American High School Students in Project Seed at Rider University, NJ 2000 - 2009. • Served as Chair of FMC Black Employee Network (BEN) to assist in hiring, training and retention of African-American employees in FMC 1996 - 2006 • Served as a technical advisor (AIChE representative) to The Global ACET Project, 2007 - 2008. ACET is a collaborative effort by organizations from around the world to combat corruption in the engineering and construction industry. • Initiated programs within FMC that provided numerous scholarships and valuable internships for African-American students 1996 - 2009. • Guest Speaker at the 50th commemoration of United Nations Human Rights Celebration at the Germantown Academy, PA, 1999. • Led many diversity initiatives in FMC. Made significant contributions as a member of the Diversity Balanced Scorecard Committee in 1999 which produced a report that Larry Brady (CEO, FMC) praised as excellent work and distributed as a model for the rest of the corporation. • Served as the FMC liaison officer on ”Project Seed” program with Rider University from 1996 to 2009. (The goal of ”Project Seed”, an ACS program, is to increase minority participation in science and engineering.) • Chaired the NOBCChE Delaware Valley Chapter STEM program from 1990 to 1994 where we adopted Overbrook High School in Philadelphia, PA to teach the students SAT on weekends that resulted in higher SAT scores that translated to record high numbers of admissions to colleges and scholarships to the students.

SELECTED PROFESSIONAL ADVANCED TRAINING IN USA

• The Fauske and Associates, Inc., ”Chemical Process Relief System Design Seminar” , Presented by Dr.

Joseph C. Leung, Burr Ridge, IL, March 13-15, 2002. • AIChE continuing education course in, ”Methods for Sizing Pressure Relief Vents”, New Orleans, LA, March 11-12, 2002. • AIChE continuing education course in, ”Engineering Design for Process Safety”, Newport Beach, CA, February 4-8, 2002. • AIChE continuing education course in, ”Hazard and Operability (HAZOP) Studies for Process Safety and Risk Management”, Philadelphia, PA, September 23-25, 2002 • AIChE Continuing Education Program on ”Mathematical Modeling and Optimization”, Houston, TX, March, 1997. • AIChE Continuing Education Program on ”Practical Project Economic Evaluation, Capital and Operating Cost Estimation”, Houston, TX, March, 1997. • AIChE Continuing Education Program on ”Use of Spreadsheets For Chemical Engineering Calculations”, Miami Beach, Fl, November, 1995 • AIChE Continuing Education Program on ”Prevention, Management and Compliance for Hazardous Wastes”, Chicago, IL , November, 1990 • AIChE Continuing Education Program on ”Fate and Transport in the Environment-Chemodynamics”, Chicago, IL, November, 1990 • Continuing Education Series on ”Advances in Emulsion Polymerization and Latex Technology”, Emulsion Polymers Institute, Lehigh University, Bethlehem, PA, June, 1990 • AIChE Continuing Education Program on ”Supercritical Extraction”, San Francisco, CA, November, 1989 • Comprehensive Zenger-Miller Frontline Leadership Course at the Mercer County Community College, NJ from September to October, 1999 • FMC Financial Management Course, Philadelphia, PA October 6 – 7, 1999

RELEVANT PUBLICATIONS PATENTS: (1) Dada, Emmanuel; Lapham, Donald; Richards, Joseph, ”Rapid Dilution of Peracid Solutions to Equilibrated Solutions”, US Patent 8,029,693 B2, assigned to FMC, October 4, 2011 (2) Dada, Emmanuel; Lapham, Donald, ”Acqueous Peracid Solutions and Stabilization Method”, US Pat Appl. Publ. US 2010/0021558 A1, Jan. 28, 2010 (3) Sethi, Dalbir; Dada, Emmanuel; Hammack, Kevin; Zhou, Xinliang, ”Auto-oxidation production of hydrogen peroxide via oxidation in a microreactor.” US patent 7,416,718 assigned to FMC, 2008

(4) Sethi, Dalbir; Dada, Emmanuel A; Hammack, Kevin; Zhou, Xinliang, ”Auto-oxidation production of hydrogen peroxide via hydrogenation in a microreactor. ” US patent 7,547,430 B2 assigned to FMC, 2008 (5) Adeniyi Lawal, Emmanuel A. Dada, Woo Young Lee, and Henry Pfeffer, ”Production of hydrogen peroxide from hydrogen and oxygen.” U.S. Pat. Appl. Publ. (2006), 17pp. CODEN: USXXCO US 2006233695 A1 20061019.

(6) Dada, Emmanuel A. ; Lau, Willie; Merritt, Richard F.; Paik, Yi H.; Swift, Graham ”Process for preparing low molecular weight polymers”, US Patent 5,328,972 assigned to Rohm and Haas

SELECTED TECHNICAL PAPERS: (1) Matthew N. O. Sadiku, Emmanuel Dada, Kazeem Olanrewaju, and Sarhan M. Musa, ”Big Data in Healthcare”, International Journal for Research in Applied Science and Engineering Technology, IJRASET, Volume 6, Issue VI, June 2018 (2) Kazeem B. Olanrewaju, Liem Thai, and Emmanuel Dada, ”Application of Computational Fluid Dynamics (CFD) in Biotransportation of Complex Fluid in the Human System”, International Journal of Scientific and Engineering Research, IJSER, Volume 9, Issue 6, June 2018

(3) Mathew N. O. Sadiku, Emmanuel Dada, and Sarhan M. Musa, ”Emerging Computing Technologies-Part 1”, CSCE’18, The 2018 World Congress in Computer Science, Computer Engineering & Applied Computing, July 30 – August 02, 2018, Las Vegas, ND, USA

(4) Mathew N. O. Sadiku, Emmanuel Dada, and Sarhan M. Musa, ”Emerging Computing Technologies-Part 2”, CSCE’18, The 2018 World Congress in Computer Science, Computer Engineering & Applied Computing, July 30 – August 02, 2018, Las Vegas, ND, USA

(5) Kazeem B. Olanrewaju, Liem Thai, and Emmanuel Dada, ”Fluid-Structure Interaction in Human Physiological System: A Computational Approach”, NOBCChE (National Organization of Black Chemists and Chemical Engineers) Conference, Orlando, Florida, September 17 – 20, 2018

(6) Emmanuel A. Dada, Kazeem Olanrewaju,”Development of CO2-Enhanced Oil Recovery in Light Tight Oil Production”, NOBCChE (National Organization of Black Chemists and Chemical Engineers) Conference, Orlando, Florida, September 17 – 20, 2018

(7) Brittani Turner, Thi Pham, Adebola Sule, and Emmanuel A. Dada,”Analysis of Recent Accidents in the Universities Laboratories: Root Causes, Lessons Learned and Prevention” , NOBCChE (National

Organization of Black Chemists and Chemical Engineers) Conference, Orlando, Florida, September 17 – 20, 2018

(8) Lisandro Fernando, Stephanie Burrs, Emmanuel Dada, ”Tight Oil Drilling Problems and Solutions”, NOBCChE (National Organization of Black Chemists and Chemical Engineers) Conference, Minneapolis, MN, November 1, 2017.

(9) Oladimeji Odusote, Adewale Lawal, Diala Olariche, Emmanuel Dada, ”Promoting Green Supply Chain Model for Sustainable Petroleum Refining”, NOBCChE (National Organization of Black Chemists and Chemical Engineers) Conference, Minneapolis, MN, November 1, 2017.

(10) Adekunle Ajike, Damian Efetobore, Emmanuel Dada, ”Smart Manufacturing in Distillation”, NOBCChE (National Organization of Black Chemists and Chemical Engineers) Conference, Minneapolis, MN, November 1, 2017.

(11) Hypatia Keys, Thi Pham, Emmanuel A. Dada, ”Integrating Safety Cultures and Practices in Research Laboratories and Manufacturing Plants”, NOBCChE (National Organization of Black Chemists and Chemical Engineers) Conference, Minneapolis, MN, November 1, 2017.

(12) Matthew N. O. Sadiku, Adebowale E. Shadare, Emmanuel Dada, Sarhan M. M, ”Smart Cities”, International Journal of Scientific Engineering and Applied Science (IJSEAS),2016, 2(10), 41-44.

(13) Matthew N. O. Sadiku, Adebowale E. Shadare, Emmanuel Dada, Sarhan M. M, ”Digital Divide”, Journal of Multidisciplinary Engineering Science and Technology (JMEST); 2016, 3(10), 5661 - 5663.

(14) Matthew N. O. Sadiku, Adebowale E. Shadare, Emmanuel Dada, Sarhan M. M, ”Physics of Failure: An Introduction”, International Journal of Scientific Engineering and Applied Science (IJSEAS), 2016, 2(10), 108 - 111.

(15) Emmanuel A. Dada, Irvin W. Osborne-Lee, Michael Gyamerah, Kazeem Olanrewaju, ”Development of Energy Efficient Process for the Capture of CO2 from Post-Combustion Coal Fired Power Plant Flue Gases Using a Novel Solvent”, Carbon Management Technology Conference, Sugar Land, TX , Nov 25, 2015.

(16) Emmanuel A. Dada, Adewale Lawal, Olariche Diala, ”Analysis of Green Supply Chain Model for Sustainable Petroleum Refining”, Carbon Management Technology Conference, Sugar Land, TX , Nov 25, 2015.

(17) Emmanuel A. Dada, Kazeem Olanrewaju, Roy A. Drayton, ”Efficient Capture of CO2 From Pulverized Coal Fired Plants”, Paper 702f, AIChE Annual Conference, San Francisco, LA, Nov 7, 2013

(18) Chike Okechukwu, Bal Shrivastava and Emmanuel A. Dada, ”A Case Study Of Debottlenecking Strides In A Petrochemical Plant”, Paper 450c, AIChE Annual Conference, San Francisco, LA, Nov 6, 2013

(19) Emmanuel A. Dada, Thomas Mensah, Derrick K. Rollins Sr., Lisa Jackson, Levi T. Thompson and Yusuf G (Debo) Adewuyi, ”The Impact of Environmental Pollution and Clean-up Technologies on the US Economy and Sustainability”, Paper 824b, AIChE Annual Conference, San Francisco, LA, Nov 4, 2013

(20) Emmanuel A. Dada, Thomas Mensah, Derrick K. Rollins Sr., Lisa Jackson, Levi T. Thompson and Yusuf G (Debo) Adewuyi, ”The Impact of New Oil Fracking Technology on the US Economy”, Paper 824c, AIChE Annual Conference, San Francisco, LA, Nov 4, 2013

(21) Emmanuel Dada, John Erinne, Oluwafemi Taiwo, ”Nigeria: Chemical Engineering- Development, Challenges and Prospects”, CEP, June 2013 (22) Emmanuel A. Dada, Azizul Azri Mustaffa and Rafiqul Gani, ”Production of Dialkly Carbonates Via Reactive-Extractive and Pressure-Swing Distillations Using Unifac-Cl VLE Model Predictions”, Paper 324d, AIChE Annual Meeting, Pittsburgh, PA, October 30, 2012. (23) Emmanuel A. Dada, Thomas Mensah, Derrick K. Rollins, Paula Hammond, Antonio Garcia, Irvin Osborne-Lee, ”Engineering Technology for Food and Health”, AIChE Annual Meeting, Pittsburgh, PA, October 29, 2012 (24) Emmanuel A. Dada,Thomas Mensah, Derrick K. Rollins, Paula Hammond, Antonio Garcia, Irvin Osborne-Lee, ”The Global Issues on Water Resources, Infectious Diseases, and the Impact of Ecological Footprint”, AIChE Annual Meeting, Pittsburgh, PA, October 29, 2012 (25)

Emmanuel A. Dada, Luke Achenie, ”Production of Cyclohexane from Hydrogenation of Benzene using Microreactor Technology”, In I.A. Karimi and Rajagopalan Srinivasan (Editors), Proceeding of the 11th International Symposium on Process Systems Engineering, 15 - 19 July 2012, Singapore. Elsevier, B.V.

(26) John C. Prindle, C. B. Panchal, Richard D. Doctor, Emmanuel A. Dada, Aspi Kolah, Carl T. Lira, Dennis Miller, ”Heat Integrated Reactive Distillation of Mesityl Oxide Process”, AIChE Spring National Meeting, Houston, TX, April 4, 2012

(27) Emmanuel A. Dada; Chandrakant B. Panchal, Richard D. Doctor, ”Heat Integrated Reactive and Extractive Distillation for the Synthesis of Carbonates in Emerging Markets ”, AIChE Annual National Meeting, Minneapolis, MN, October 2011.

(28) Emmanuel Dada, Thomas Mensah, Derrick K. Rollins, L. Antonio Estévez, Otis Shelton and Joycelyn Harrison,” Lessons Learned from and Economic Impacts of Fukushima, Japan Disaster”, Paper 99a, AIChE Annual Meeting, Minneapolis, MN, October 2011.

(29) Emmanuel Dada, Thomas Mensah, Derrick K. Rollins, L. Antonio Estévez, Otis Shelton and Joycelyn Harrison,”The STEM Education and Its Impacts On Pipeline for Underrepresented Minorities”, Paper 99b, AIChE Annual Meeting, Minneapolis, MN, October 2011.

(30) Chandrakant B. Panchal, Vyjayanthi Alagharu, Emmanuel Dada, Chris C. Thomas, ”Process Intensification of Multi-Effect Evaporation and Crystallization”, AIChE Spring National Meeting, Chicago, IL, March 15, 2011

(31) Aspi K. Kolah, Venkata K.S. Pappu, Carl T. Lira, Dennis J. Miller, Emmanuel A. Dada, C.B. Panchal, Richard D. Doctor and John C. Prindle, ”Heat Integrated Reactive Distillation for the Indirect Hydration of Cyclohexene to Cyclohexanol”, AIChE Annual National Meeting, Chicago, March 2011

(32) Kolah, Aspi K. Lars Peereboom, Carl T. Lira, Jing Huang, C.B. Panchal, Robert W. Lyczkowski, Emmanuel A. Dada, Richard D. Doctor and Dennis J. Miller, ”Advanced Reactive Distillation Concepts for the Indirect Hydration of Cyclohexene to Cyclohexanol”, Paper 77c, AIChE Spring Meeting Chicago, IL (March 15, 2011)

(33) Panchal, Chandrakant B. , John C. Prindle, Jing Huang, Robert W. Lyczkowski, Richard D. Doctor, Emmanuel A. Dada, Philip Lutze, Rafiqul Gani and John M. Woodley,”Heat Integrated Reactive Distillation”, Paper 107g, AIChE Spring Meeting, Chicago, IL (March 16, 2011)

(34) Emmanuel A. Dada; Chandrakant B. Panchal, Richard D. Doctor,”Production of Dimethyl Carbonate Via Reactive Distillation Process”, AIChE Spring National Meeting, Chicago, IL, March 2011

(35) Philip Lutze, Rafiqul Gani, John M. Woodley and Emmanuel A. Dada, ”Recent Advances in Reactive Distillation”, 40th NSChE (Nigeria Society of Chemical Engineers) Annual Conference/AGM Port Harcourt, Nigeria November 18 - 20, 2010

(36) Philip Lutze, Rafiqul Gani, John M. Woodley and Emmanuel A. Dada, ”Recent Advances in Reactive Distillation”, Paper 539C, AIChE Annual Meeting, Salt Lake City, UT (Nov 11, 2010)

(37) E. A. Dada, R. D. Wesson, C. Grant, D. K. Rollins, G. A. Barabino, ”The Pipeline for Future Engineers and Its Impact on US Competitiveness”, Paper 128b, AIChE Annual Meeting, Salt Lake City, UT (Nov 8, 2010)

(38) Philip Lutze, Rafiqul Gani, John M. Woodley and Emmanuel A. Dada, ”Recent Advances in Reactive Distillation”, NOBCChE (National Organization of Black Chemists and Chemical Engineers) Conference, University of Pennsylvania, Philadelphia, PA, November 6, 2010

(39) Philip Lutze, Emmanuel Dada, Rafiqul Gani, John M. Woodley, ”Heterogeneous Catalytic Distillation-A Patent Review”, Recent Patents on Chemical Engineering, 2010, 3, 208-229

(40) Emmanuel A. Dada, Rosemarie D. Wesson, L. Antonio Estevez, Thomas Mensah, Victor Atiemo-Obeng, Christine Grant, Tom R. Marrero, ”The Pipeline for Future Engineers and its Impact on US Competitiveness”, Paper 69b, AIChE Annual Conference, Nashville, TN, November 9, 2009

(41) Emmanuel A. Dada, Rosemarie D. Wesson, L. Antonio Estevez, Thomas Mensah, Victor Atiemo-Obeng, Christine Grant, Tom R. Marrero, "Perspectives on the Energy Challenges Facing the US Including Impacts on Sustainability", Paper 69c, AIChE Annual Conference, Nashville, TN, November 9, 2009.

(42) Emmanuel Dada, "Overview of MAC-AIChE College Scholarships for Underrepresented Minorities in Chemical Engineering", AIChE Annual Meeting, Philadelphia, PA, Nov. 16-21, 2008

(43) Emmanuel Dada, Dalbir Sethi, and Dayi Deng, "Production of Hydrogen Peroxide via the Direct Combination of H2 and O2 in a Pilot Microreactor." AIChE Spring National Meeting, New Orleans, April 7, 2008.

(44) A. Lawal, R. Halder, S. Tadepalli, Y. Voloshin, H. Chen, W. Y. Lee, and E. Dada, "Microchannel Reactor System Design & Demonstration for On-site H2O2 Production by Controlled H2/O2 Reaction," Invited Presentation, Process Intensification Topical Conference, AIChE Spring National Meeting, April 13, 2005 (45) Emmanuel Dada, "Supercritical Water Oxidation Technology as an Alternative to Incineration for Hazardous Wastes Treatment", at 34th NSChE Annual Conference/AGM Port Harcourt, Nigeria November 24- 27, 2004.

(46) A. Lawal, W. Y. Lee, and E. Dada, "Microchannel Reactor System Design & Demonstration for On-site H2O2 Production by Controlled H2/O2 Reaction," Invited Presentation, Process Intensification Topical Conference, AIChE Spring National Meeting, April 2, 2003. (47) Reid, Michael H.; Dada, Emmanuel A., "Recovery of Alcohols during Esterification", AIChE Spring Meeting, New Orleans, LA, USA, March 2002. (48) Dada, E.; Lau, W.; Merritt, R. F.; Paik, Y. H.; Swift, G. "Synthesis of poly (acrylic acid) acids in super-critical carbon dioxide." Polymeric Materials Science and Engineering (1996), 74, 427. (49) Dada, E.; Lau, W.; Merritt, R. F.; Paik, Y. H.; Swift, G. "Synthesis of poly (acrylic acid) acids in super-critical carbon dioxide." , 211th ACS National Meeting, New Orleans, LA, March 24-28 (1996) (50) Dada, Emmanuel A; Wenzel, Leonard A., "Adsorption of binary liquid mixtures of amines on zeolite 13X at 29 degree C.", Journal of Chemical and Engineering Data (1991), 36(3), 319-21. (51) Dada, Emmanuel A.; Wenzel, Leonard A., "Estimation of the adsorbent capacities from the adsorption isotherm of binary liquid mixtures on solids." Industrial & Engineering Chemistry Research (1991), 30(2), 396-402.

SPECIAL RESEARCH PROJECTS REPORTS 1. "Waste Heat Recovery and Recycling in Thermal Separation Processes: Distillation, Multi-Effect Evaporation (MEE) and Crystallization Processes," DOE EE0003479, (Emmanuel A. Dada; Chandrakant B. Panchal; Luke K. Achenie; Aaron Reichl; Chris C. Thomas), ( www.osti.gov/servlets/purl/1056308/ ), U. S. Department of Energy, December, 2012. 2. Several Internal Proprietary reports at FMC and Rohm and Haas on production of hydrogen peroxide, biodeggradable polymers, and peracetic acid applications and development.

FUNDED RESEARCH PROJECTS AND CONSULTATIONS (1) Irvin W. Osborne-Lee (PI) and Emmanuel A. Dada (Co-PI) a $20K Research Mini Grant, College of Engineering, PVAMU on Development of Energy Efficient CO2 Capture from Coal Fired Plant Flue Gases, May – August 2015 (2) Richard Doctor (PI), Chandrakant B. Panchal (Co-PI) and Emmanuel A. Dada (Co-PI) a $1.1 million 2-year DOE funded research on Argonne National Lab project Heat Integrated Reactive Distillation, July 2010-September 2011. (3) Emmanuel A. Dada (PI) and Chandrakant B. Panchal (Co-PI) a $300K 1-year DOE Funded Grand Challenge FMC Project on Waste Heat Recovery on August 2010 to January 2012. (4) Consultant to E3TEC Services on $120K 9-month DOE SBIR Project on Heat Enhancement Process Intensification of Multi-Effect Evaporation and Crystallization January 2010 - August 2010. (5) Consultant to CPT on $1.7 million DOE funded research awarded to Stevens Institute of Technology on microreactor technology applications to pharmaceutical and allied industries. April 2003 - August 2008. (6) A. Lawal (PI) and Emmanuel A. Dada (Co-PI) a $1.5 million DOE funded research awarded to FMC and Stevens Institute of Technology on a novel microchannel reactor design for the production of hydrogen peroxide by the direct combination of hydrogen and oxygen. April 2002 to August 2007. (7) Consultant to Safe Foods Corporation, Arkansas on Production of Peracetic Acid, Dec 2016-present (8) Submitted two proposals to NSF on STEM in collaboration with Univ. of Iowa and PVAMU, 2017

SUMMARY OF RESEARCH AND TEACHING INTERESTS

Research Interest

• To carry out research in the areas of process improvements in shale oil/tight oil and gas. To investigate and provide solutions on the impacts of water resources in shale oil and gas development. • To develop and demonstrate innovative technological improvements for the capture and subsequent use of CO2 from coal and gas-fired flue gas from power plants and other sources to substantially reduce the greenhouse gas effects and environmental pollution. • To develop energy efficient processes across chemical and petroleum industries. The applications of heat integrated reactive distillation and other separation techniques to achieve significant energy and cost savings will be developed including the separation of close boiling olefins and paraffin. Energy recovery from waste heat will be investigated. • To actively carryout research for the application of fundamental thermodynamic principles and kinetics to advanced oxidation processes (sonochemistry, etc) for reduction of pollutants like NOx, SO2, VOC, and Hg. • To use computer aided softwares like ASPEN , HYSIS and ICAS in process and product development and in modeling the underlying principles and behavior of new routes to products of interest . (ICAS is Integrated Computer Aided Software developed by Prof. Rafiqul Gani of Technical University of Denmark whom I have collaborated with for many years.) • To build on my collaborative research activities with other faculty members in my university and other universities, government sponsored research entities (NSF, DOE, etc) for effective research in different areas and to form and/or participate in research center(s) as appropriate. • To encourage my undergraduate students to do research with me and interest them in STEM education especially with the goal to increase the participation of underrepresented minorities in science and engineering fields.

Teaching Interest

My extensive industrial experience prepares me to teach several courses in the chemical, biochemical, and environmental engineering programs in both undergraduate and graduate level courses. In particular, my industrial experience prepares me to teach senior capstone design course using examples from my industrial background for the senior projects which I have supervised senior projects from 2012 to present at PVAMU. I would like to develop new undergraduate and graduate courses in alternative and clean energy, process safety, engineering project management, innovation in oil and gas exploration and emergent technologies. I will demonstrate and show genuine interest to help my students in doing their best in their courses, encourage them to participate in class discussion and have open door policy on office hours for my students and complement with virtual office hours using SKYPE and others. Use the course assessment results to improve my teaching skills and use of innovative technologies when available with practical industrial examples to aid students in better understanding of the courses that I teach. Using computer aided software like ASPEN, HYSIS and ICAS to complement teaching aids. Provide my students with useful and reliable references on links on YOUTUBE on relevant technology and courses. I would also like to collaborate with the faculty in the internationally recognized Mary Kay O'Connor Process Safety Center of TAMU to teach process safety to both undergraduate and graduate students.

MASTER PROJECTS SUPERVISED AT PRAIRIE VIEW A & M UNIVERSITY 1. Nana Adjapong, "Deep Water Developments via Subsea Flow assurance", December 2014 2. Adeola Adetunji, "A Review on Carbon Dioxide Capture Approaches from Coal Fired Power Plant", May 2015 3. Kingsley Ejiofor, " Enhanced Oil Recovery via Carbon Sequestration", May 2015 4. Olariche Diala, "A Review on Carbonate Looping for CO2 Capture in Power Plants", Dec. 2015 5. Ripal S. Joshi, " Environmental Air Permit Application for Ethylene Manufacturing Plant Expansion: A Case Study", May 2016 6. Joseph Maduabuachi, "Impact of Climate Change on USA Economy", May 2017 7. Adebola Sule, "Analysis of Recent Accidents in the Universities Laboratories", August 2017 8. Lisandro Fernando, "Tight Oil Drilling Problems and Solutions", December 2017

UNDERGRADUATE PROJECTS SUPERVISED AT PRAIRIE VIEW A & M UNIVERSITY Supervised undergraduate student (Rodney Smith) research in 2016 Supervised 3 undergraduate students (Adekunle Ajike, Hypatia Keys and Thi Pham) research in 2017.

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**Session XXXX**

# Artificial Intelligence (AI) in Chemical Processes
# ASEE GSW Annual Conference Paper

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## Abstract

Artificial Intelligence (AI) is an area of computer science that accentuates the development of programs that enable computer systems and machines to perform tasks that usually need human intelligence and reactions. This implies that AI could eventually replace human input. Most chemical industries use computational methods such as simulation design and optimization for their processes; an area where AI could excel. AI could provide a significant impact in problem-solving, mathematical analysis, and information technology by optimizing processes in chemical industries. AI has been widely used in various applications of the chemical engineering field including modeling, process control, classification, fault detection, and diagnosis. AI has promising applications in new areas that include materials design such as catalysts, nanostructures, pharmaceuticals, additives, polymeric composites, rubber compounds, and alloys. Also, machine learning (ML), an area of AI has been used to integrate physical models and computational techniques for autonomous molecular design in the chemical and pharmaceutical industries, especially in the manufacturing of soft bio-inspired materials [35].
In this paper, we explained AI in general, analyzed the logic behind AI, identified promising current and future opportunities of AI application in chemical industries, where AI can be implemented to enhance operations in chemical industries, and how to increase the efficiency of chemical processes. An extensive literature review on applications of AI in the chemical industries was also carried out. With the advent of relatively easy-to-use software like Python, the barrier to implementing AI has significantly come down.

Keywords: Artificial Intelligent, Machine Learning, Deep Learning, Chemical Processes

## Introduction

The Logic Theorist was the first Artificial Intelligence (AI) developed in 1955 by Hertbert Simon and Allen Newell. Since then, a lot of progress has been made, also with the broad growing reach of Machine Learning (ML) into different areas is easier to build an AI solution than it was before. Al is expected to create $13 trillion jobs by 2030. Although people fear Al taking their jobs, according to accountancy firm PwC, over 7 million jobs will be displaced by AI between 2017 and 2037. However, it will also lead to the generation of 7.2 million jobs, which is a net gain of 200,000 jobs, and Chemical processes/Industries will be part of this job loss and gain [36].

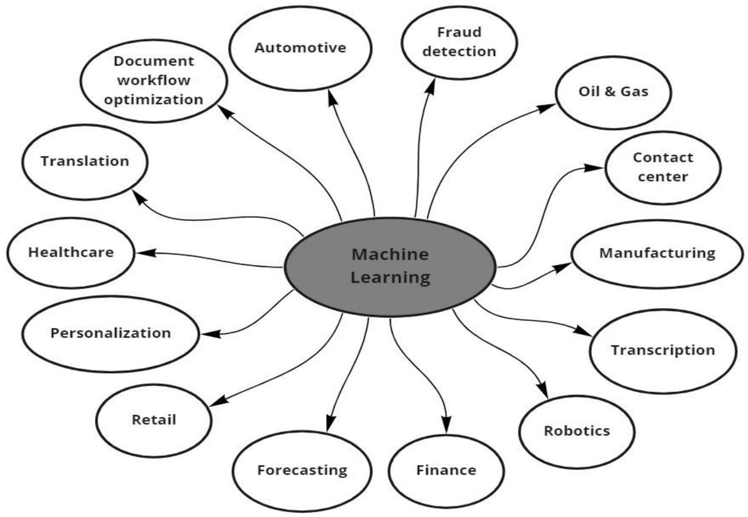


**Figure 1: Machine Current Reach**

Building AI architecture and acquiring skills needed for AI will help both the industry and engineers to keep innovating and solving problems. ML, deep learning (DL), and big data are important parts of AI. In chemical engineering, Al has been used in fault detection, chemical substance detection, modeling, optimization, and material design as a catalyst. Solving nonlinear function approximation and nonlinear classification problems in an automated manner, using the backpropagation learning algorithm was a breakthrough that fostered much research in AI. The objectives of this paper are to explain AI in general and analyze the logic behind AI, identify promising current and future opportunities of AI application in chemical industries, where AI can be implemented to enhance operations in chemical industries, and how to increase the efficiency of chemical processes through AI implementation.

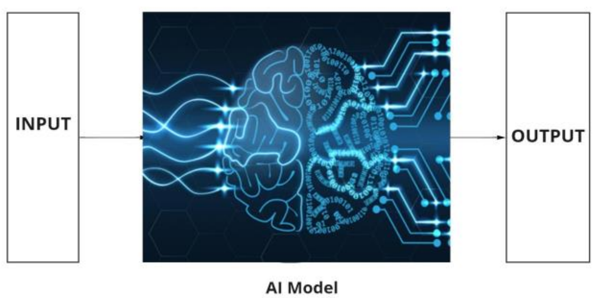


**Figure 2** AI Model (Modified from [30])

## Stages of AI in the chemical process industry

In general AI in chemical process industries can be categorized into different stages: Zero Stage (Early Strive), First Stage (Expert System Era), Second Stage (Neural Networks Era), Third Stage (Deep Learning and Data Science Era), and Fourth Stage (Self-Supervised Learning) future.

*A. Zero Stage (Early Strives) before 1983*

Since data and data structures are a particularly important part of AI, this was believed to be the time a system applied AI methods such as means-and-ends analysis, symbolic manipulation, which linked data structures in chemical engineering. Also, the Adaptive Initial Design Synthesizer system developed for process synthesis was a significant development.

*B. First Stage (Experts System Era)*

This era is the time when system programs imitate the problem-solving skills of humans with the expertise in an input area based on knowledge-based, rule-based, or production systems, typically heuristics model of learned and refined over times of problem-solving experience. The architecture of these systems was inspired by the stimulus-response model of cognition from psychology and the pattern-matching-and-search model of symbolic computation, which originated in Emil Post's work in symbolic logic [3]. The production system framework was introduced during this era. This allowed for flexible execution, and it also facilitated the incremental addition of knowledge, without distorting the overall program structure. This rule-based knowledge representation and architecture are intuitive and relatively easy to understand and generate explanations about the system's decisions. This system applies a clear distinction between the knowledge base and the search or inference strategy. This led to unique developments like:

- MYCN for infectious diseases diagnoses.
- PROSPECTOR for mineral prospecting.
- CONPHYDE for predicting thermophysical properties of complex fluid mixtures. DECADE for catalyst design.
- DESIGN KIT MODELLA for developing process models.

The current Clean Energy Smart Manufacturing Innovation Institute which was founded in 2016 was as a result of a large-scale program in this era. Also, the Abnormal Situation Management (ASM) consortium was funded at $17 million by the National Institute of Standards and Technology's Advanced Technology Program and by the leading oil companies, under the leadership of Honeywell [34]. Venkatasubramanian (Columbia University, New York), Davis (Ohio State) group leader, and Vicente (University of Toronto), were the three academic groups, also involved in the consortium [3].

*C. Second Stage (Neural Networks Era)*

Neural Networks Era was the great turning point era from the top-down design paradigm of expert systems to the bottom-up paradigm of neural nets that acquired knowledge automatically from large amounts of data, as a result easing the maintenance and development of models. Backpropagation algorithm reinvention started it all in this time where the process of training feedforward neural networks to learn hidden patterns in data input-output started by Rumelhart, Hinton and Williams in 1986. The ability to solve nonlinear function approximation and nonlinear classification problems in an automated manner using the backpropagation learning algorithm was the breakthrough in this era.

Nonlinear modeling automation skills helped researchers make considerable progress on addressing challenging problems in modeling [14,15], fault diagnosis [16-21], control [22,23], and product design [24]. Acknowledgment of Kramer, Bakshi, and Stephanopoulos's great work respectively in the connection between the autoencoder architecture and the nonlinear principal component analysis

[14], and the identification of the nature of the basis function approximation of neural networks through the WaveNet architecture [15]. Also, success was made in expert systems here based on ASM consortium and genetic algorithms. First this birthed evolution of engineering polymers in silico using genetic algorithms led to the multiscale model-based informatics framework called Discovery Informatics [27] for materials design. That also led to the successful development of materials design systems using directed evolution in several industrial applications such as gasoline additives [28], formulated rubbers [28], and catalyst design [29]. AI systems such as Prodigy and Soar were also developed. From 1990 to 2008, face recognition, vision, natural language processing, and speech recognition were not solved in this era due to the lack of many layers of neural nets.

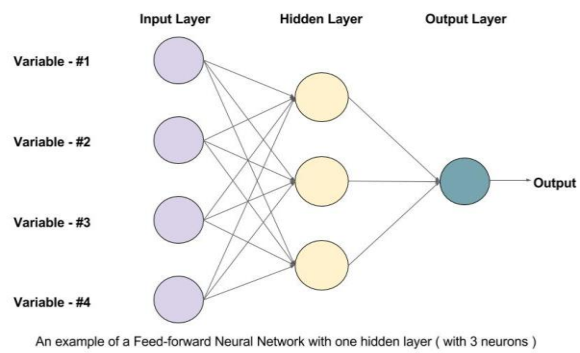


**Figure 3:** Feed-forward Network (Source:[31])

*D. Third Stage (Deep Learning and Data Science Era) Present*

Deep learning is a subfield of machine learning that structures algorithms in layers to create an artificial neural network that can make intelligent decisions on its own through learning while Machine Learning is the ability to learn without being explicitly programmed. These vital ideas made this stage of deep learning or convolutional neural nets (CNNs), reinforcement learning, and statistical ML possible. These are the technologies that are behind the recent AI success stories in game playing, natural language processing, robotics, and vision.

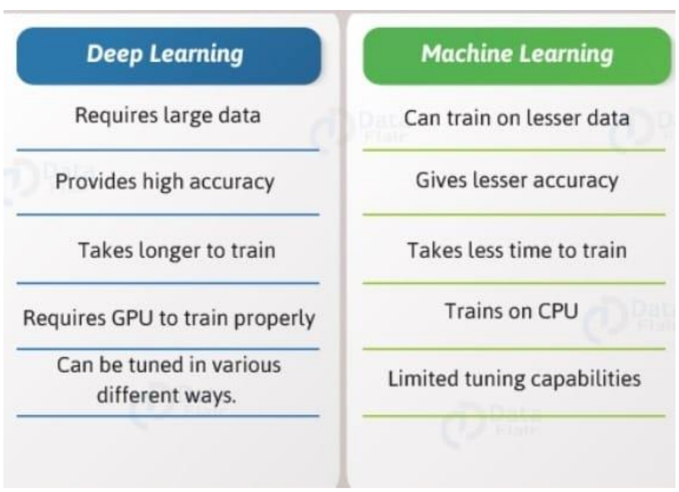


**Figure 4:** DL AND ML Capability (Source: [33])

A **CNN** from a large data set learns during training, which is a key requirement, by the network, the appropriate filters that lead to a successful performance. Also, **Recurrent neural network** (RNN) architectural innovation, where connections between nodes form a directed graph along a temporal sequence, is designed to understand data characteristic sequence and use patterns to predict the next likely scenario. Used in speech recognition and language processing. Later, the **long short-term memory** (LSTM) unit innovation was invented. The normal LSTM unit is made of a cell, an input gate, an output gate, and a forget gate. The cell remembers values over arbitrary time intervals and the three gates regulate the flow of information into and out of the cell. LSTM networks are well suited for making predictions based on time series data since there can be lags of unknown duration between important events in a time series. **Reinforcement learning**, which has positive and negative reinforcement learning can be thought of as a scheme for learning a sequence of actions to achieve the desired outcome, such as maximizing an objective function. An example is AlphaG which can be used in process improvement and optimization.


**Figure 5:** Reinforcement Learning in ML architecture (Source: [32])

**Supervised learning** is where the system learns the bond between input (X) and output (Y) given a set of input-output (X-Y) pairs. This means a set of training samples and labeled training data consistently in a function. Likes of regression algorithms and classification algorithms are supervised learning.

**Unsupervised learning** is where we have clustering unsupervised learning algorithms that can be used in the training set that has no artificially labeled results. Useful methods such as LASSO, Support Vector Machines, random forests, clustering, and Bayesian belief networks came from **Statistical ML** which is the combination of mathematical methods from probability and statistics with ML methods. In this stage, problems in synthesis, design, control, scheduling, optimization, and risk analysis, were solved by modeling human information processing and decision making. Also, fault diagnosis and process hazards analysis that require causal model-based reasoning are better addressed by AI concepts and techniques.

*E. Fourth Stage (Self-Supervised learning Era) Future*

This is believed to be the next stage of AI. Basically, going by the same logic that animals and humans learn extremely fast, through observations. The likelihood approach is predicting everything from everything else, training a system to predict the missing information by filling in the gab. If a system can accurately predict what is going on in a live process in terms of product defects, hazards or breakdown, it will help drive efficiency, productivity and reduce industry risk. This is case by case in which automated data labeling and human interaction are eliminated. In self-supervised learning, the learning model trains itself by leveraging one part of the data to predict the other part and generate labels accurately.

## Applications of AI

*The following are some of the applications of AI:*
*Application of AI in chemical process modeling* using ANN and fuzzy logic in modeling processes such as catalyst deactivation in reactors.
*Application of AI in optimization* using the best solution from various alternatives of operating variables, to maximize or minimize the desired objective to reduce cost and increase value.
*Application of AI in fault detection and diagnosis:* Fault detection and diagnosis have been the focus of many researchers over the years. The utilization of neural networks to identify faults is becoming increasingly sought after in the chemical industry. Neural networks have a high potential for capturing nonlinear relationships. Neuro-fuzzy diagnosis applications in chemical plants are proposed in the literature [8-9].
*Chemical Process Modeling:* Hybrid Mamdani Fuzzy and Genetic Algorithms (GA) Zelnab Hajjar.
*Chemical Process optimization*: Generic population-based metaheuristic optimization algorithm based on evolutionary algorithms (EAs) like GA [12], harmony search [13], and particle swarm optimization.
*Neural Network Control:* Adaptive neuro-fuzzy inference system (ANFIS) controller is a hybrid intelligent system approach that uses the learning ability of the neural network with the knowledge representation of the fuzzy logic for chemical performance improvements. Furthermore, Inverse model control is the input vector for a neural network that required future and reference output together with past inputs and the past output variables, which can lead to better performance in controlled variables when the unmeasured disturbance is present. The carefully adjusted variable of the controlled plant is the output neural network controller [3].
*Property and Activity (Toxicity) prediction:* Used Quantitative structure-activity/property relationship analysis (QSAR/QSPR) involves regression and classification model [Zeren Jiso, 2020]
Consequence Analysis: The development of ML algorithms, the artificial neural network (ANN) has been mostly used in consequence prediction like gas dispersion and source terms estimations. It could also be overcome the limitation of missing source information in emergency cases by integrating it with other dispersion models such as PHAST or FLACS. The backpropagation neural network to correlate the detected gas concentration was developed by Wang et al. [10] So hazardous gas dispersions could be estimated even when the source information is unknown. NI et al. To solve the conflict between accuracy and efficiency requirements of the gas dispersion model, deep belief networks (DBNs) and convolution neural networks (CNNs) was introduced. NI et al.

*These are some of today's pertinent ML structures and domains:* TensorFlow, PyTorch, Pylearn2, Scikit-learn, Deeplearning4j, MATLAB (MatconvNet MATLAB DL), Keras, Caffe, Caffe2, Theano, Lasagne and Blocks, MXNet, Chainer, CNTK, Torch, DL toolbox and Opentrons OT-2 with an open-source.
The presence of Python and Automated ML made programming applications and integration ML architecture very much easier.

In chemical process industries, AI can be applied in Consequence Analysis. The biggest limitation of ML-based consequence analysis is the lack of experimental data since it is extremely expensive and hazardous to conduct field dispersion experiments. The use of Virtual and Augmented Reality (VR/AR) to help the simulation generate data for model training and validation is recommended. Also, the simulation tools can take account of complex environmental parameters that can highly influence the consequence. Unlike using HYSYS and other similar simulators that do not have the capability. Natural language processing of archived data and reports can assist risk assessment.[11] Image recognition can identify potential safety hazards and operation abnormalities.

## Conclusion

Many great applications have been developed that are ready to produce quick successes in this new data science phase of AI with applications in chemical industries. However, the interesting and intellectually challenging problems lie in developing such conceptual frameworks as hybrid models, mechanism-based causal explanations, domain-specific knowledge discovery engines, and analytical theories of emergence. AI still has a lot to offer chemical industries and some shortfalls could be offset using first-principles knowledge wherever possible and building hybrid AI systems, which can impose some rigor and discipline on purely data-driven models, which could lead to more breakthroughs.

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