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The Sustainable Path towards Polymers and Nanomaterials: A Researcher's Insight

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In recent decades, increased environmental concerns to reduce carbon foot print and rising prices of petrochemicals have attracted much attention towards developing green and sustainable biodegradable polymers and nanomaterials, which will help in securing the planet's ecological balance. The studies based on utilization of renewable resources for development of value-added products ensuring environmental sustainability have become essential to confront the unprecedented implications of petroleum-based products related to global warming. Nature-based nanomaterials such as cellulose nanocrystals (CNCs), are derived from the abundantly available cellulosic biomass with unique inherent characteristics that have led to increased scientific and industrial attention. CNCs are the crystalline domain of cellulose with rod-like morphology and interesting properties such as high surface area, tunable aspect-ratio, chemical functionality, anisotropic mechanical properties, self-ordering behaviour to form optically active materials along with improved biocompatibility, biodegradability and non-toxic nature, provides it an upper hand in comparison to other nanoparticle derivatives. CNCs due to its sustainable nature, bio-origin and anisotropic mechanical behaviour have promising applications as reinforcing agents in polymeric nanocomposites, as targeted drug delivery vehicles, in biocatalysis, and in paper-based electronics as sensors. However, production of CNCs through industrially viable approach is still a challenging task due to high processing time, uncertainty in initial cellulosic precursor and requirement of stringent acid hydrolysis conditions. Moreover, literature survey suggests that processing of CNC-based polymeric nanocomposites through scalable extrusion techniques results in agglomeration due to their hydrophilic nature alongwith severe degradation in the molecular weight of polymer. Therefore, the present doctoral thesis aims to address both the techno-economic challenges associated with the processing of CNCs or its polymeric composites and develop advanced functional materials with CNCs as building block for high performance applications.

In the present work, CNCs have been fabricated from renewable feedstock such bamboo stems, rice husk, commercial pulp and newspaper for their potential application as commercially viable value added products, with a strategy to convert "wastes to wealth". The challenges associated with high production time was overcome with an indigenously developed CNC production unit coupled with continuous dialysis system which reduces the processing time to ~24-26 hours in comparison to ~7 days through traditional approach. Interestingly, CNCs with tunable physico-chemical, structural and morphological properties, are fabricated by simply varying the initial cellulose polymorphism or the type of acids used as hydrolyzing agents, explicitly during its processing step. Strategic modification of CNCs through this sustainable approach avoids the utilization of harmful and toxic chemicals which might affect the biocompatible and non-toxic properties of CNCs. Dispersion of surface-modified CNCs into polymeric matrix leads to the formation of percolation network which results in considerable improvement of mechanical and barrier properties of biodegradable polymers (such as polylactic acid (PLA) and polyhydroxybutyrate (PHB)), making them ideally suited for food packaging applications. An industrially viable approach for processing PLA/CNC films through reactive extrusion process have been developed which was successfully tested on a pilot-plant scale extruder in presence of wide range of compatibilizers. The reactively processed PLA/CNC cast films shows improved molecular weight characteristics, thermo-mechanical and barrier properties with dimensional stability and migration values within the standard limits, which is generally difficult to achieve through traditional extrusion process limiting their commercial viability. The developed

films are promising for food packagings and result in improved self-life of ~5 months and ~2 weeks respectively for the storage of oil and dairy based products. In addition, these films have the potential to be produced at commercial scale through utilization of industrial scale extruders with improved dimensional stability, stable molecular weight and physico-chemical characteristics. Magneto-responsive CNCs, are one of the versatile nanomaterial which have been developed in this work, with potential applications as self-propagating nanobots with autonomous motion as targeted drug delivery vehicles, biocatalysts with high activity and as templates for fabrication of graphene nanoscrolls with tunable geometry and encapsulated metallic nanoparticles as hydrogen storage devices. Magnetic field directed alignment of such nano-block units introduces anisotropic thermo-mechanical, electrical and magnetic properties alongwith the hyperthermia characteristics finds potential applications in development of bio-inspired materials with microstructural features comparable to biological materials for high performance engineering applications. Therefore, the research work of the author was mainly focused on functionalization of CNCs for development of polymeric bionanocomposites as well as their advanced functional derivatives and studying their efficacy in sustainable chemical processes with targeted opportunities for their commercial scale production.

Mathematical modeling of micro photosynthetic power cells: A short review

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Abstract:

Micro-photosynthetic power cell (μ PSC) is one of the bio-electrochemical systems which acts as both an energy harvesting and an energy conversion device. Development of μ PSCs requires expertise from the areas of biology, chemical, mechanical and electrical engineering. Mathematical modelling of μ PSCs is complex as its working is linked to several interacting phenomena and factors. In this article, the need for mathematical modelling, challenges involved, and the progress in the development of mathematical models for μ PSCs are provided. First principles (lumped and distributed parameter) models and the electrical equivalent circuit models for μ PSCs in literature are briefly reviewed.

1. Introduction

Micro-photosynthetic power cell (μ PSC) is a niche energy harvesting technology which can be used for low-power to ultra-low power applications such as lab on chips and wireless sensor networks [1]. Micro-photosynthetic power cell (μ PSC) is a bio-electrochemical device that generates power by harvesting the energy from light and also by the metabolism of products of photosynthesis. Due to this unique feature, μ PSC can generate power in both dark and in the presence of the light.

This article is organized as follows. First, a brief introduction to the history of the development of μ PSCs is presented followed by the working of μ PSCs. Next, the need for the development of mathematical models, challenges involved in the development of mathematical models are presented. Finally, recent progress in the mathematical modelling of μ PSCs is reviewed.

1.1 Background

μ PSCs are a miniaturized version of photo-microbial fuel cells (Photo MFCs). Photo-MFCs are a category of microbial fuel cells (MFCs) in which the photosynthetic micro-organisms are employed. Depending on the place where the photosynthetic micro-organisms are employed and based on whether they are employed either separately or in conjunction with the other micro-organisms, photo-MFCs are divided into several categories [2]. Photo-MFCs in which photosynthetic organisms are employed in the anode chamber alone and with an electron acceptor in cathode chamber are termed as photo electrochemical cells (PECs) or photosynthetic power cells (PSCs). Early research on MFCs and photo-MFCs involved the use of large volumes of anode and cathode chambers [3]. Miniaturized versions of both MFCs (μ PSC) and micro photo-electrochemical cells (μ PSC) are introduced as a potential power sources for the applications which require low powers (tens of micro-watts). Lam et.al [4] first proposed μ PSC; the power generated was in the order of nano-watts. With the progress in research on μ PSCs, there has been a significant improvement in the amount of the power produced due to improved designs and more appropriate materials.

1.2 Working of μ PSCs

A μ PSC, like all other electrochemical cells, comprises of anode and cathode chambers with a membrane electrode assembly (MEA) sandwiched between them. The anode chamber contains photosynthetic

organisms in the nutrient medium to support its growth and a mediator to shuttle electrons and protons from bulk of the anode chamber to anode electrode surface. In the cathode chamber, the electron acceptor is present, which receives the electrons from the anode chamber. The fabrication procedures and materials used for different components of μPSC varies across various designs reported till now [4–9]. A dual chamber μPSC developed by Shahparnia et.al. [9], the components and its working are shown in Figure 1.

2. Need for mathematical modeling of μPSCs :

Even though there has been progress in the performance of μPSCs , this area is still in a nascent stage of development. The performance of μPSCs depends on several factors such as the photosynthetic organism, mediator, and the electron acceptors solutions used. Further, the design of μPSC and operating conditions such as pH , light intensity and temperature etc., can also influence the performance. One can improve the performance of μPSCs by understanding the influence of these factors and their interactions on the functioning of μPSCs . Mathematical modeling can aid in understanding the influence various design parameters, operating conditions and also to enhance performance of μPSCs through identification of optimal designs and operating conditions.

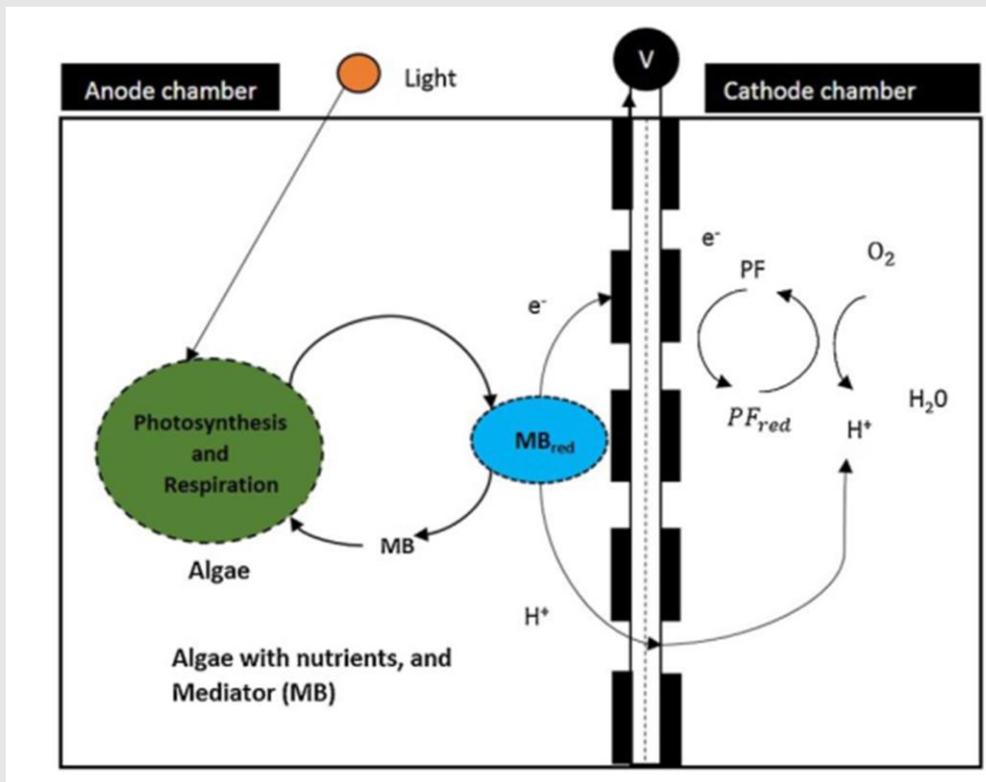


Figure 1: Working of micro photosynthetic power cell. Anolyte: Chlamydomonas reinhardtii with Sueoka's High Salt Medium (HSM) and Methylene blue mediator. Catholyte: 25% Potassium ferricyanide. MEA: Nafion with Gold (100 nm) patterned on both sides. During photosynthesis and respiration, electrons and protons are released in the electron transport chains of photosynthetic microorganisms are siphoned by mediator in its reduced form to the anode surface. Reduced mediator releases protons and electrons at the anode and converts back to its original form. Electrons travel through the external circuit generating current. Protons travel through Nafion membrane to the cathode chamber. Potassium ferricyanide gets reduced to potassium ferrocyanide at the cathode surface. Potassium ferrocyanide combines with protons and the dissolved oxygen in cathode chamber to form water. (Taken from [11])

3. Challenges involved in mathematical modeling of μ PSCs:

It is evident from the literature that studies that are reported on μ PSCs are mostly dedicated to fabrication and improvement of performance through different designs and use of different materials for the components of μ PSCs [4]–[9]. Even though it is useful to develop mathematical models to help in design and operating conditions optimization, research in this aspect of μ PSCs is minimal. Reasons for this could be two-fold. First, s are a quite new and emerging area. Hence, the focus is on development of new devices. The second, mathematical modeling of systems such as μ PSCs is extremely complex. The challenges involved in development of mathematical models for μ PSCs are presented next.

Challenges involved in the development of mathematical models for μ PSC:

μ PSC comprises of the anode chamber, a MEA, and the cathode chamber as major components. Accurately modeling the phenomena occurring in these components is challenging due to the complexity and interactions involved.

Reactions inside the anode and cathode chambers are bulk reactions and the reactions occurring at the surface of electrodes (anode and cathode) are electrochemical reactions. Ideally, to model the bulk reactions in the anode chamber of μ PSCs, mathematical representations for photosynthesis, respiration and their interactions are needed. Since, photosynthesis and respiration themselves are complex processes and depend on parameters such as design of the anode chamber, light intensity, P^H of the chamber and concentration of photosynthetic organisms etc., it is hard to obtain simple mathematical equations representing those processes.

In addition to this, to model the kinetics of photosynthetic species, biological models are needed. Further, to model the diffusion of the mediator and its reduced form, spatial variation of concentrations of these components (results in partial differential equations) is to be considered in the bulk of the anode chamber.

Similarly, in the bulk of the cathode chamber, the spatial variation of concentrations of an electron acceptor and its reduced forms is to be considered to model their diffusion. All the phenomena discussed till now characterizes the reactions occurring in the bulk of the anode and cathode chambers. Additionally, development of electrochemical equations to model electrode reactions at the anode and cathode surfaces and modeling the proton exchange membrane considering the fluxes of species transported through it based on electrochemical reactions add more complexity to mathematical modeling of μ PSCs. Hence the development of mathematical models for μ PSCs is really challenging and needs expertise in several disciplines.

4. Review of mathematical models of μ PSCs

Mathematical models that are developed to date for μ PSCs are lumped parameter and distributed parameter models by Tanneru et.al. [10,11] and the electrical equivalent circuit models (ECMs) by Masadesh et.al. [12] and Tamanwe et.al. [13].

The lumped parameter model developed by Tanneru et.al. [10] was the first and a simple model for the μ PSCs. The main assumption made in this model development was to ignore the spatial variation of the concentration of species, and the phenomena that are not explicitly modelled are lumped into one parameter. The difficulties involved in modelling of the phenomena in the anode and the cathode chambers are mitigated by using the representative reactions at the anode and cathode surfaces. These reactions were developed based on the working of μ PSC and mechanisms of photosynthesis and respiration.

Since the diffusion of the species were not explicitly considered, these phenomena were captured in the lumped model parameter (k). This k was designed as a function of rates of representative reactions at the anode and cathode (k_a , k_c) and the charge transfer coefficient α . The model parameters were obtained through minimizing the RMSE error between the experimental data from Shahparnia et.al. [9] and model predicted voltage. The model was validated from the experimental data that was not used to obtain model parameters. The developed model was able to predict the – characteristics of the μPSC s. This model was used to perform the sensitivity analysis on the operating parameters such as light intensity, electrode surface area and the concentration of algae. The developed model demonstrated the power of a simple model by providing insights in to the different operating regimes of a μPSC even though those phenomena were not explicitly modelled.

As a continuation and improvement to the lumped parameter model of Tanneru et.al [10], a distributed parameter model was proposed by Tanneru et.al.[11]. In this model, the spatial variation of concentration of species in the anode and the cathode chamber were considered using 1-D diffusion along the depth of the chambers. Few model parameters are taken from literature and the rest are obtained from experimental data reported by Shahparnia et.al.[9]. The developed model was used for performing sensitivity analysis on the design parameters electrodes areas, depth of the chambers to obtain the optimal aspect ratio that improves the performance of a μPSC . The proposed model was also used to obtain optimal current and voltage to be drawn from the single μPSC and the number of μPSC s connected in series for a required power through explicit optimization formulations.

Since the power generated by μPSC s is intermittent, energy harvesting circuits are needed to optimally harvest the power from them. The use of first principles models in development of energy harvesting circuits would be computationally intensive. Therefore, ECMs of μPSC s are generally used for this purpose. Masadeh et.al.[12] developed first ECM of μPSC s. The model parameters are obtained from experimental data of Ramanan et.al. [8] and Shaparnia et.al. [9]. The model performance is validated by comparing the model predicted – charactersitics and the dynamics responses of the μPSC s for different loads with the experimental data of Shaparnia et.al. [9]. Prior to Masadeh et.al.s' work, Ramanan et.al. [8] had used curve fitting technique to obtain the relationship between voltage and current of the μPSC s and simulated the performance of 2 μPSC s connected in series and parallel. Tamanwe [13] has recently developed energy harvesting circuit along with the development of ECM for μPSC .

Summary:

A brief introduction to one of the emerging technologies that can be a power source for low power applications, μPSC , is provided. The need for mathematical model development, and challenges involved are explained. The current status of research on mathematical modelling of μPSC s is provided by briefly reviewing the existing mathematical models. Note: Authors request the readers to consult the full papers to appreciate model formulation, solution approaches, model validation and the usefulness of the models in design and optimization of μPSC s.

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Safer handling of self-reactive hazardous chemicals in chemical manufacturing plant

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Fire and explosions are very common in the chemical reactor of process industries, specially the one involved in handling organic peroxides used as initiators, hardeners or cross-linking agents [2] during polymerization and azo compounds which have a frequent usage in the fields of medicine, paint, rubber, cosmetics, foodstuffs etc [4]. Both these group of compounds grab attention in any catastrophic disaster owing to the presence of relatively weak and unstable bond between the oxygen atoms (-O-O-) in organic peroxide and bivalent bonding of the nitrogen atoms (-N=N-) which can be ruptured easily as in azo compounds. The feature of reactivity for these self-reactive chemicals can be attributed to the breakage around the weak single or double bond to undergo radical or ionic decomposition. The cleavage around the bond is brought by the proximity of external thermal source which releases large amount of heat and subsequently it is affected by rapid temperature and pressure rise. The decomposition reactions are exothermic in nature with high activation energy and their kinetic studies which have deduced them to be temperature sensitive; cannot be sensitized at ambient temperature, though the rate of reaction becomes significant at higher temperature [7]. This phenomenon eventually triggers the runaway reaction, more so, if the heat-generating rate is more than the heat-removal rate; it leads to deadly fire, thermal explosion, and toxic release of gas causing severe pollution to the environment. These groups are incompatible with materials like acid, base, metal ion and contaminants. A violent reaction in the manufacturing process initiates on adding an acid or alkaline catalyst. This brings in a huge release of energy and many fatalities have been reported due to human error while adding incorrect feed ratio or inappropriate kinetic assumption. In 2014 Kaohsiung, Taiwan explosion disaster was caused by propylene gas.

Cumene hydroperoxide (CHP) is used as an initiator for polymerization to produce acrylonitrile-butadiene-styrene (ABS) resin. It is produced when cumene is oxidized in presence of aqueous sodium carbonate. 94.5% of CHP is used to produce phenol with acetone in a catalytic reaction [1].

Benzoyl peroxide (BPO) is a non-toxic, colorless, odorless and tasteless crystalline solid. It is very unstable, initiator of polymerization, acts as a bleaching agent and degrades to form benzoic acid by free-radical mechanism [3].

Methyl ethyl ketone peroxide (MEKPO) is produced by reacting methyl ethyl ketone (MEK) with hydrogen peroxide (H_2O_2). It is used as a radical source for initiation and it acts as a cross-linker during polymerization. MEKPO is inherently unstable which can decompose even in an ambient atmosphere and hence demands precaution in handling and storage.

AIBN (2, 2'-Azobisisobutyronitrile) is commercially used alkyl azo compound, used as an initiator in polymerization. It slowly breaks down even at room temperature so it should be placed below $10^{\circ}C$ and presence of any external heating source should be avoided [6].

Various studies have been conducted on organic peroxide and azo compounds group of chemicals keeping in mind the explosion and catastrophic incidences caused by them according to Table 1. Calorimetric tool like DSC determines the basic thermo kinetic data like exothermic onset temperature (T_0), peak temperature (T_{max}) and enthalpy of reaction like (ΔH_d) under non-isothermal or dynamic mode. TAM III was used for determining the decomposition under isothermal condition and the incompatibility effect of acid, base or alkalis and contaminants on the chemicals was used to obtain the thermo kinetic

data like TMR_{iso}, time of reaction. VSP2 application helped to investigate these chemicals to evaluate their maximum self-heating rate $(dTdt^{-1})_{max}$, maximum pressure rise rate $(dPdt^{-1})_{max}$ and time to maximum rate under adiabatic condition (TMR_{ad}). TIC (thermal imaging camera) was used to study azo compound and a peroxide group of chemical namely CHP mixed with incompatible alkaline solution. TIC can be used to ascertain runaway reaction in providing information such as about the storage, phase-transformation of reactive compounds. The qualitative estimation of the products obtained on decomposition of reactive chemicals has been analyzed with GC/MS studies [5]. The results of these studies aim to provide safety information commencing from the manufacturing process till establishment of an emergency relief conditions under disturbed atmosphere.

Table 1: Selected incidents of fire or explosion caused by organic peroxides and azo compounds.

Date	Chemical	Location	Injuries	Fatalities	Cause
2000.08.24	MEKPO	Korea	11	3	Unknown
2000.08.24	BPO	USA	1	0	Thermal decomposition
2000.08.24	AIBN	China	59	21	Thermal explosion (storage tank)
2000.08.24	ABVN	China	5	42	Thermal decomposition
2000.08.24	Propylene	Taiwan	310	32	Pipeline gas leak

ABVN: 2,2'-azobis-(2,4-dimethylvaleronitrile)

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A Peek into Artificial Intelligence, Machine Learning and Data Science

Priya Choudhary

A look back in history

Often regarded as the fourth industrial revolution, Artificial Intelligence and its related fields of Machine Learning and Deep Learning isn't a new concept to mankind. Although common in talks today thanks to the many ways it touches human life, the research has been ongoing since decades. So what has the journey been like? It has been less than a century ago, that with the development of technology, especially the electronic and stored program computer AI has taken off from imagination to plausible reality. Much of the success is widely credited to British prodigy Alan Turing, who in the 1950's pioneered the idea of giving machines the ability to think, just like humans. In his paper, Computing Machinery and Intelligence he discussed the techniques to build and test intelligent machines, which has helped propel research and discussions in this area till date.

The highs and lows

With the improved functionality and accessibility of computers the wheels had further set in motion, work in AI field had flourished fueling enough for the next fifty years. The research community also improved in formulation and application of machine learning algorithms such as deep learning in the 1980's. Although the theory being in place, due to lack of funding significant computational power there were certain phases of dormancy in between. Despite the enhancement, computers yet weren't capable enough to contain data or process it fast enough to be of practical intelligence. There was still a long way to go before the end goals of natural language processing, abstract thinking, and self-recognition as known today could be realized.

Moving forward, during the 1990s and 2000s, many of the landmark goals of artificial intelligence had been achieved. Though the coding and theory hadn't got any smarter, what had changed was the fundamental limit of computer memory and speed holding back decades before, having finally caught up and in many cases surpassing our needs. This is precisely how Deep Blue was able to defeat Gary Kasparov in 1997, and how Google's Alpha Go was able to defeat world Go champion, Lee Sedol in 2016. This offers a bit of an explanation to the roller coaster of AI research has been through time.

AI in Present Day

Currently, in 21st century we live in the age of 'Big Data' which refers to the data presents in immense volume, high velocity and variety which cannot be processed with traditional applications. However, today the computational power and infrastructure is well developed to help collect huge sums of data and has the ability to crunch numbers to draw powerful insights. Some example of popular sources of these data sets would from media, IOT devices and the Web. The very premise of AI technology is its ability to constantly learn from the data it collects. The further data there is to gather and analyse through carefully crafted algorithms, the enhanced the machine becomes at making predictions.

What does the future hold?

In the immediate future, AI is the next big thing. In fact, much of it is already underway and affects us in daily lives such as online recommendations and ads, or perhaps interacting with a chat bot. In the long run, the landscape could possibly be changed by driverless cars and the goal is commonly spoken as general intelligence, where a machine could possibly surpass a human's cognitive abilities in all tasks.

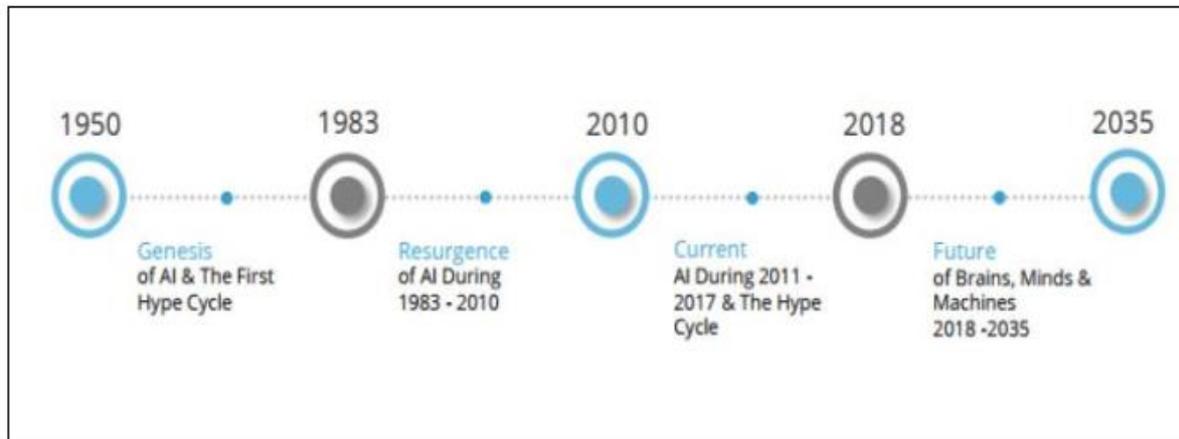


Figure 1. A timeline summary of the phases in AI [Ref: scrvanalytics.ai]

So how is Machine Learning or Data Science related to Artificial Intelligence?

There exists a good amount of overlap in the three fields, however are not exactly identical. One of the brief and simplified definitions to classify them is as follows

- Artificial Intelligence helps produce actions
 - AI is considered an evolution of this first encounter between math and computer science, and primarily tries to simulate of the human brain function by machines, by achieving logical reasoning, learning and self-correction.
 - Modern Artificial Intelligence is often broken into two areas: General Artificial Intelligence and Applied Artificial Intelligence.
 - General AI pertains to making machines intelligent in a wide array of activities that involve thinking and reasoning, this is where most of the exciting advancements are taking place today. This is also the area that has directed to the development of Machine Learning.
 - On the other hand, Applied AI involves the use of artificial intelligence for a very specific task such as maneuver an autonomous vehicle.
- Machine Learning helps produce predictions
 - The difference between Artificial Intelligence and Machine Learning is a bit more subtle, and historically ML has often been considered a subfield of AI, or an application of AI on idea that given data access to machine, it should be able to learn patterns and gain intelligence.
 - Designing systems that can change responses based on the data used for training. As they are exposed to more data, they become efficient, scalable and adaptable for certain applications compared to those explicitly programmed by people.
 - Commonly explained with “given instance X with certain features, help predict the outcome Y”. Hence, it is the ability of machine, such as computer to learn from environment and improve with time as more experience is gained by the system
 - It has been achieved through the development of numerous algorithms over the past fifty years, which learn from data provided, gather insights and make predictions on new information helping understand possible future outcomes.
 - The algorithms have been classified in three basic models of learning, Supervised, Unsupervised and Reinforcement Learning.

- Data science produces insights
 - AI and ML fall under the realm of computer science, DS is distinguished from the other two fields because the end goal is an especially human one: to gain insight and understanding.
 - As the classic definition of data science as an inter-disciplinary combination of statistics, software engineering, and domain expertise, it emphasizes on human skills of statistical inference, experiment design, data visualization, domain knowledge and communication, apart from expertise on relevant tools and technology.
 - Having said that, though DS isn't exactly a subset of ML, it uses ML to analyse data and make predictions, combined with big data analytics and cloud computing.
 - There would always be a human element to assess whether the predictions made in ML phase does truly add value or is random output. Hence, the domain expert's discretion is required in understanding the insight, seeing the figure, or benefitting from the conclusion.
 - In a nutshell, Data science is a practical application of machine learning with a complete focus on solving real-world problems, such as sales forecasting or spam detection.

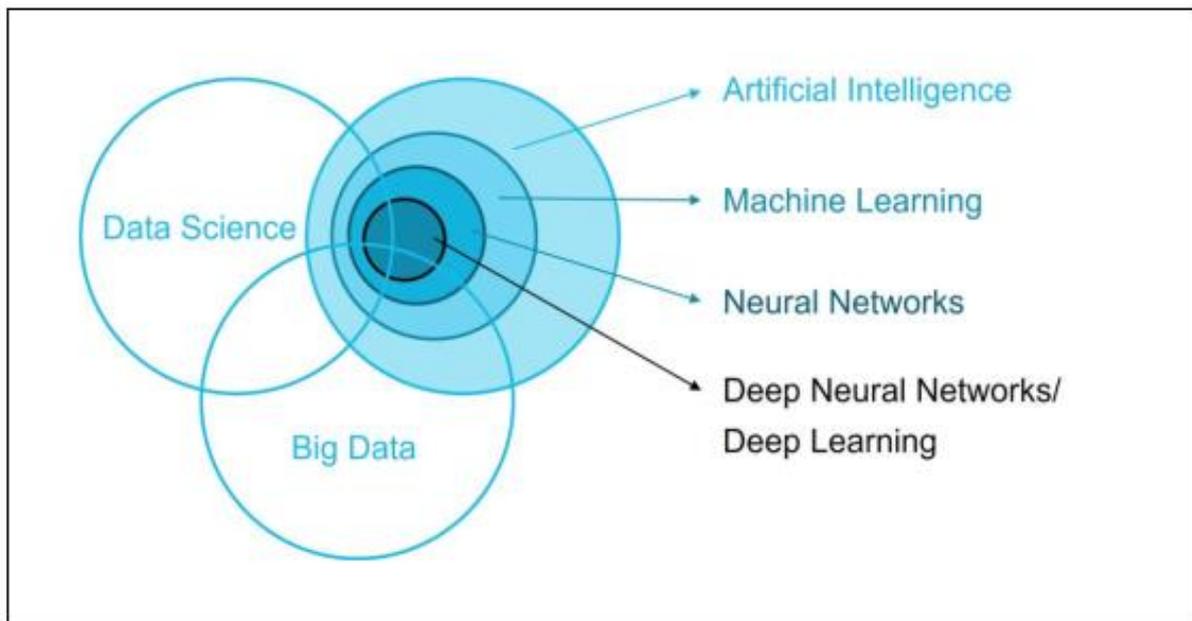


Figure 2. Venn diagram explaining the overlaps in the various fields [Fraunhofer FOKUS]

Summary

As depicted in the Venn diagram, there are various subsets of Artificial Intelligence, each having a different intersection with the various other fields. In the AI preview, it is Machine Learning which has gained significant popularity by being able to nearly transform science fiction to become a daily reality. Few other areas of AI such as Natural Language Processing and Robotics are equally popular. Further within Machine Learning, among the plethora of algorithms developed, Deep Learning which incorporates neural networks has outperformed not only classical methods but also human benchmarks with impactful applications such as image and speech recognition.

Additionally, as it can be seen Data Science isn't exactly a subset of Machine Learning however, the integration of ML and DS is when the learning happens with help of training data, which commonly involves leveraging big data techniques to fine tune a model or algorithm parameters. The main difference being that DS covers the whole spectrum of data processing and visualization, combining the algorithmic or statistical aspects of ML with a complete focus on solving real-world problems. Hence, broadly speaking it has been the right interplay of these fields in creating the new revolution which captures human imagination.

References:

1. <https://courses.cs.washington.edu/courses/csep590/06au/projects/history-ai.pdf>
2. McCorduck, Pamela (2004), Machines Who Think (2nd ed.), Natick, MA: A. K. Peters, Ltd. ISBN 1-56881-205-1, OCLC 52197627
3. <https://intelligence.org/files/EthicsofAI.pdf>

Seminar Series on *Can Supercapacitors surpass Batteries for Electric Mobility*

Dr. S. A. Ilangovan, Group Director, Chemical Systems, Vikram Sarabhai Space Centre, delivered this talk on November 1, 2018.

Seminar Series on *Electrocatalytic oxidation of arsenite using Pt based electrodes*

Prof. Hasnat, Shajalal University of Science and Technology, Bangladesh, delivered this talk on November 26, 2018.

Kinetics of electrocatalytic oxidation of arsenite ions has been investigated at a Pt disk electrode using cyclic voltammetry, convolution potential sweep voltammetry and electrochemical impedance spectroscopy. A complimentary environment pertaining to oxidation reactions of arsenite ions is attained in the acidic medium compared to a neutral or basic medium. It is suggested that in the neutral and basic media, direct electron transfer from the solution to electrode instigate the oxidation process without any pre adsorption. Meanwhile, in the acidic medium, prior to oxidation, arsenite ions are adsorbed on the Pt surface and a stepwise reaction mechanism is involved. Using impedance analysis, it is suggested that different forms of surface oxides at various pH values control the oxidation kinetics.

Seminar Series on *Co-ordination assisted self-assembled nanostructure: a Futuristic Engineered nano-formulation for advanced therapeutic application*

Prof. Santanu Chattopadhyay, Rubber Technology Centre, Indian Institute of Technology, Kharagpur, delivered this talk on December 24, 2018.

Co-ordination assisted self-assembly of the macromolecules is one of the unique approaches to achieve a stimuli-responsive monodispersed

nano-formulation (NF) applicable in biomedicines. The stimuli-responsive structural reorganization property of these NF's draws an enormous attention in the field of NF based biotherapy. Herein we came up with two different types of smart-formulation showing stimuli-responsive structural deformation followed by their therapeutic performance towards the specific biological environment. Firstly, the macromolecule, pentaerythritol poly(caprolactone)-b-poly(acrylic acid) form Fe³⁺ ion induced light-responsive NF with the unique structural arrangement as like spherically shaped human brain. The DOX-loaded NF undergoes structural deformation in the presence of light and shows a release of DOX molecule (85.2% at 120 min). Administration of the DOX-loaded NF to C6 glioma rat model (in vivo) offered tremendous inhibition (~91%) of tumor growth without any toxic side effects. Secondly, mannose conjugated antimicrobial polypeptide, poly(arginine-r-valine)-mannose undergoes Zn²⁺ ion induced self-assembly into a NF with a unique structural appearance as like *Taxus baccata* fruits.

The NF uptake by the bacterial membrane led structural deformation followed by exposing of free polypeptide molecules. These molecules are enforced to lysis the bacterial membrane followed by diffusion of cytoplasmic component out of the membrane that culminates final death of bacteria (MIC values varies from 0.67 to 2.55 μ M). Indeed, NF's remain non-toxic against both the mammalian as well as red blood cell as reflected from their higher order of cell viability (> 80%) and very insignificant hemolytic effect (<13%). Hence, metal ion assisted self-assembly approach brings about a new therapeutic window, where the fully exposed macromolecule can be formulated into compact NF with enhanced therapeutic performance.

Industry-Academia Interface Seminar on Upstream Petroleum Engineering

Indian Institute of Chemical Engineers - Guwahati Regional Centre and the Department of Chemical Engineering, IIT Guwahati conducted a half day Industry-Academia Interface Seminar titled "Upstream Petroleum Engineering" on November 10, 2018 (Saturday). The following lectures were delivered by resource persons from industry and academia.

- Lecture on "Fundamentals of Petrophysics" by Prof. Archana Nair, Department of Civil Engineering, IIT Guwahati.
- Lecture on "Reservoir Management" by Mr. Manish Kumar, Oil India Limited
- Lecture on "Pressure Transient Analysis" by Mr. Bhaskar Bhargav, Gas Authority of India Limited
- Lecture on "Enhanced Oil recovery" by Mr. Debashish Baishya, Oil India Limited

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