SHORT SERIES

THE ENERGY CONSORTIUM
IIT MADRAS

ACCELERATING NET ZERO

PREFACE

The consortium is leading the transition to net zero through technology and accelerating the rate of adoption of new technologies. This makes The Energy Consortium, the country's preeminent Energy organization.

When we think of developing net zero technologies and innovation then there is no better microcosm of the world than India. It is a crucible of every kind of a test situation that a technology would experience in the entire world. We have pockets in India that are so well developed that they would possibly mimic any western European context, and then there are also pockets of India that are very green and forested remote islands providing a context of other parts of the world. As a microcosm we believe, this is a great place to come and experiment for technologies that would help the whole world become net zero.

The idea of net zero and climate change is a very unique problem that has been posed for the first time in our civilizational journey. Never before has mankind experienced a global scenario that requires a global solution with survival at stake. This presents us with a situation where we really have to look at technologies in a global context with adoption and efficacies of technologies also in a global context and India is providing that kind of context. Technologies that are either developed in India or those that are developed elsewhere but test-bedded in India will provide the right kind of feedback and answers for the world context.

At IITM we have been focused on energy related technologies for several decades and the overall ecosystem that we have out together, in terms of faculty, in terms of research infrastructure, the innovation culture, and the student driven ecosystem are all the reasons why one will see energy research going that much farther.

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EDITOR'S NOTE

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The Energy Consortium was founded in Dec 2021 with a bold vision: to enable India's journey towards a low carbon energy future. In this short span, we have eleven global energy majors, that include those in hard to abate and hard to electrify sectors as well as those at the forefront of leveraging digital means for energy transition, collaborating with us. We are now participating heavily in two major alliances, one focused on energy storage and another on green fuels. We are actively partnering and advising government agencies on topics of national and international importance and have represented the cause at the COP28 in Dubai. This has allowed us to drive collective action at scale and emboldens us to contribute more assertively towards the net zero journey of India.

As per the Ministry of New & Renewable Energy data, India, at the end of 2023, became 4th globally in Renewable Energy Installed Capacity, 4th in Wind Power capacity and 5th in Solar Power capacity. We recognize that the time has come to elevate our mission. We must transition from just enabling progress to actively accelerating the realization of a net zero future. Together with our partners in industry and government, we can ensure that net zero is not just an aspiration, but an imminent reality for India and the world. Building on our vision, we are now in mission mode, fully dedicated to Accelerating Net Zero at the Energy Consortium.

In this second edition of our short series of white papers we bring together seminal topics that are going to shape how we accelerate achieving net zero.

I am glad to have the real world perspective from a global energy leader, Aramco, available to our readers. A perspective that provides extremely insightful and vital commentary on the need as well as approach that organizations and governments must take to realize at-scale deployment of carbon capture and its utilization or storage.

Further, and given the central role played by the electric power grid in our ability to meet energy transition targets, we are happy to include an authoritative overview article that speaks about the electrical power markets and how they are undergoing a rapid transformation during the digital divide and energy transformation.

Finally, we have two progressive updates, one on the role of computing for developing clean energy technologies and another on the ability of heating and cooling solutions to significantly and favourably impact the decarbonization journey.

The global transition to a net-zero carbon economy is not just an environmental imperative but also an economic opportunity. By leading the charge in clean energy innovation and carbon capture, we are paving the way for a sustainable future that benefits both our planet and future generations.

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THE ROLE OF CARBON CAPTURE, UTILIZATION, AND STORAGE IN THE ENERGY TRANSITION

Dr. Ali A. Al-Meshari
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As a global energy leader, Aramco is driving collaboration across the world to help address some of the most pressing global challenges and support a more sustainable energy future. Aramco has a global research presence in several innovation hubs to leverage world-class scientific expertise with a view to speeding up lower-carbon energy solutions and technology development. Aramco has also recently joined the Energy Consortium at the Indian Institute of Technology Madras, with a focus towards accelerating research and innovation on lower-carbon energy technologies. By developing transformative technologies, Aramco aims to contribute to the global lower-carbon economy.

CCUS in the global energy transition puzzle

Despite the remarkable progress of renewable energies in the global energy mix and the significant improvement in energy efficiency, global greenhouse gas emissions have not decreased enough to put the world on a net-zero emissions trajectory. The urgency to act on climate, combined with the scale of ambitions to reduce global greenhouse gas emissions, means realistic approaches are needed worldwide — leveraging various potential solutions and technologies. Deployment of emerging technologies could be key towards reducing greenhouse gas emissions.

Carbon Capture, Utilization and Storage (CCUS) is a suite of technologies that can contribute to reducing CO_2 emissions from industrial facilities, as well as CO2 already accumulated in the atmosphere. As such, CCUS can help reduce emissions in key sectors such as cement, steel, and chemicals. In the cement industry specifically, about 50% of CO_2 emissions from cement manufacturing are not related to fossil fuel. A cement facility with 100% renewable electricity would therefore still release significant CO_2 into the atmosphere. CCUS value goes beyond emissions management and into opportunities to harness captured CO_2 in emerging lower-carbon businesses, such as hydrogen, e-fuels, and other lower-carbon products. Captured CO_2 could be reused or recycled, following a circular carbon economy approach.

CCUS technology is already deployed across 50 facilities worldwide, storing around 51 million tons of CO_2 in 2024, according to the Global CCS Institute. In 2024, there were 628 CCUS projects at various stages of development, an increase of about 60% from 2023. However, according to McKinsey, global CCUS capacity would still need to grow over 100 times reaching 4-6 gigatons CO_2 by 2050, to meet current announced net-zero targets.

Aramco perspectives on CCUS

CCUS aligns with our business growth aspirations and emissions reduction goals, such as Aramco's ambition to achieve net-zero Scope 1 & 2 greenhouse gas emissions across its wholly-owned operated facilities by 2050.

Aramco has robust experience in large-scale and complex engineering projects, and has also been operating one of the first large scale CCUS projects in the Gulf region since 2015, with the capacity to capture up to 800,000 tons of CO_2 per year. The CO_2 is captured from a natural gas liquefaction plant located in Hawiyah, purified, transported through an 85-kilometer pipeline, and then injected into the Uthmaniyah oil field, where it is used for enhanced oil recovery. The project is equipped with an extensive CO_2 monitoring and surveillance program, with seismic sensors to monitor the CO_2 plume and breakthrough speed.

In another project, hydrocarbons were converted to lower-carbon hydrogen, and then ammonia for export. In 2020, we demonstrated the shipment of high-grade blue ammonia

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from Saudi Arabia to Japan. The associated carbon dioxide emissions were captured and transported for utilization in two different locations: for methanol production at a SABIC facility and enhanced oil recovery at Aramco's Uthmaniyah oil field. Aramco is also involved in two demonstration plants that aim to capture CO_2 from industrial facilities, and combine it with renewable hydrogen to produce e-fuels, which are produced using renewable energy sources to generate electricity that drives the production of hydrogen via electrolysis. This hydrogen then reacts with the captured CO_2 to create liquid or gaseous hydrocarbons, substituting conventional fuels.

Additionally, Aramco has established one of the world's largest venture capital funds, Prosperity 7, through its venture capital arm Aramco Ventures, to invest in low-carbon solutions that include CCUS technologies. In 2025, Prosperity7 is expected to open an office in Bangalore, India.

Aramco is currently working with partners to build one of the world's largest Carbon Capture and Storage (CCS) hubs in Jubail, in the Eastern Province of Saudi Arabia. First phase construction is expected to capture up to 9 million tons of CO_2 from three Aramco gas plants and other industrial sources.

Aramco is also investing in CCUS research and development. Our R&D includes developing advanced materials for CO_2 capture, utilizing CO_2 in new energies and chemicals, and storing CO_2.

Enabling CCUS deployment at scale

However, the current pace of global CCUS deployment is not aligned with net-zero ambitions. The technology faces several deployment challenges, including its risk profile. These challenges are country and industrial sector dependent, but generally revolve around lack of policy support, regulatory barriers, finance, and

technology perception.

From a policy perspective, governments need to support revenue stream growth to incentivize CCUS deployment. Successful policy instruments applied to renewable energies are relevant to CCUS, such as grants, public procurement, obligations or feed-in-tariffs. The concept of a CCS hub is proving to be an effective business model for scaling-up CCUS, and governments have a key role to play in facilitating stakeholder engagement — as well as supporting CO_2 transport and storage infrastructure development.

Often, countries may also lack clear regulatory frameworks across the CO_2 value chain. CO_2 is often classified as waste, but in the era of CCUS there is a need to reconsider CO_2 classifications, streamline CO_2 storage permits, clarify long term CO_2 storage liability, and establish standards across the CCUS value chain.

Mobilizing financial resources in support of large scale CCUS projects also remains an important challenge, as many financial institutions lack clear guidelines for such projects. The finance sector should ensure CCUS is part of their climate strategies, and is eligible for sustainable finance.

Public and private stakeholders should also work together to facilitate knowledge exchange on CCUS. This involves exploring opportunities for international collaboration and strategic partnerships in CCUS technologies, along with investment opportunities.

Aramco believes CCUS may be an important component of the global energy transition puzzle, and aims to play a role in its development and deployment. With a focus on research and development, investment in a CCS hub, and collaboration with partners, Aramco aims to capture and store millions of tons of CO_2 annually, as part of its efforts to contribute to a lower-carbon future. However, deploying CCUS at scale requires overcoming several challenges. Governments, industries, and civil society must come together to overcome these hurdles to enable widespread adoption of CCUS. By working together, we can unlock new opportunities for growth, job creation, and more sustainable development.

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Industrial Heating and Cooling

HEATING AND COOLING: A DECARBONIZATION IMPERATIVE

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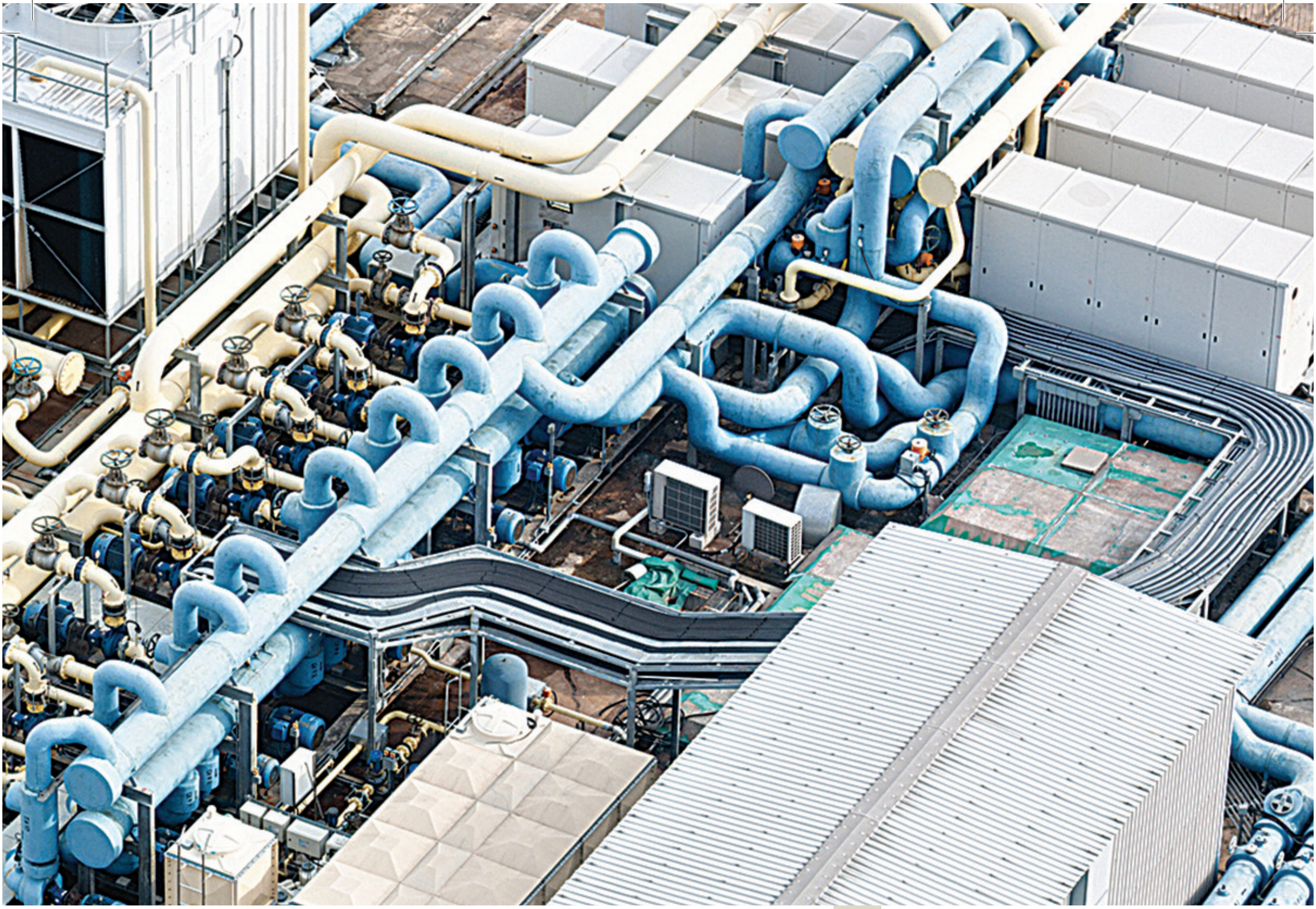

Introduction

Heating and cooling systems are central to global energy consumption, especially in industrial and domestic settings. In 2015, heating accounted for approximately 31,000 terawatt-hours (TWh) of thermal energy worldwide, primarily from fossil fuels. Similarly, the demand for cooling is rising exponentially, driven by climate change and urbanisation. Addressing these challenges requires innovative technologies and systemic changes to enable sustainable, efficient, and low-carbon solutions.

Global Demand and Challenges

Heating demand comprises industrial processes (50%), domestic space heating (45%), and smaller fractions for hot water and cooking. Before the Ukraine war, much of this demand was met with natural gas, particularly in Europe, North America, and China. The conflict underscored the vulnerabilities of fossil fuel dependence, intensifying the urgency for alternative solutions.

Cooling demand has surged as well. In 2016, the United States consumed over 620 TWh for cooling, compared to 320 TWh in 1990. In India, cooling demand, which was negligible in 1990, had risen to 90 TWh by 2016. Projections estimate an 800 GW increase in generation capacity by 2050 to meet this growing need. The increased reliance on cooling significantly strains power grids, particularly in tropical countries, where cooling can account for up to 50% of peak power demand.

The carbon intensity of energy systems exacerbates the environmental impact of heating and cooling. For example, India's grid emits 700 grams of CO_2 per kilowatt-hour (kWh) of electricity, making decarbonisation essential. Urban heat islands further compound

Countries around the world are adopting innovative strategies to decarbonise heating and cooling systems. With its hydroelectric-powered grid emitting less than 20 grams of CO_2 per kWh, Norway has significantly reduced domestic heating emissions through widespread heat pump adoption

cooling needs, creating localised hotspots that perpetuate a vicious cycle of increased energy consumption.

Decarbonisation Strategies

Electrifying heating systems is a critical first step. Traditional electric heating systems offer a coefficient of performance (COP) of around 1, meaning they convert one unit of electricity into nearly one unit of heat. In contrast, advanced systems like heat pumps achieve COP values greater than 3 by transferring ambient heat, making them significantly more efficient. Heat pumps use refrigerants to transfer heat from a cooler region to a warmer one. They offer dual functionality, providing both heating and cooling. By optimising waste heat utilisation, heat pumps can achieve COP values as high as 5, making them both economically and environmentally advantageous.

Countries around the world are adopting innovative strategies to decarbonise heating and cooling systems. With its hydroelectric-powered grid emitting less than 20 grams of CO_2 per kWh, Norway has significantly reduced domestic heating emissions through widespread heat pump adoption. Japan's "Eco Cute" program, which uses CO_2 as a refrigerant in heat pumps, has halved emissions compared to conventional electric water heaters. In the United States, cities like New York are retrofitting buildings with energy-efficient systems, leveraging heat pumps to lower emissions and energy costs. China is replacing coal-fired heating in northern cities with geothermal and solar thermal networks, reducing CO_2 emissions by millions of tons annually. Meanwhile, India is piloting solar-assisted cooling systems, such as photovoltaic-integrated systems in Gujarat, which are projected to reduce grid emissions by 40% during peak demand. These examples underscore the global shift toward sustainable heating and cooling solutions.

Transitioning to sustainable heating and cooling systems can yield substantial CO_2 reductions. Replacing coal- and natural gas-powered heating systems with heat pumps powered by renewable electricity can reduce emissions by up to 70%, with individual heat pump systems in Europe saving 2-4 tons of CO_2 annually. High-efficiency systems and waste heat utilisation can cut emissions by 30-50% for cooling. In India, where cooling demand is expected to surge, emissions could increase by 400 million tons annually if left unchecked. However, integrating renewable energy with advanced cooling technologies could mitigate more than half of this impact, significantly reducing the carbon footprint.

Technological Advancements

Technological advancements are focused on high-temperature heat pumps, refrigerants, Phase Change Materials (PCMs), and renewable integration with grid decarbonisation.

The EnERG lab, a constituent lab of the Energy Consortium at IITM, has deployed heat pump technology up to 120°C, sufficient for many industrial processes, such as food processing and textiles. Efforts are underway to develop systems capable of reaching 200°C, further expanding their applicability. On refrigerants natural refrigerants like CO_2 are gaining traction due to their low environmental impact. However, challenges such as high ambient temperatures and cost barriers must be addressed to enable widespread adoption, especially in regions like India.

To fully exploit the benefits of heat pumps, it is sometimes necessary to store thermal energy. PCMs store thermal energy by transitioning between solid and liquid states. For example, ice can store cooling energy, while wax can store heat. Efforts are on at the gas hydrates lab led by Prof Rajnish Kumar at IITM to identify suitable hydrate materials that can effectively store cooling energy at temperatures in the range of 10 – 14°C, which can significantly improve cooling systems efficiency as these operate at temperature required in the HVAC industry unlike traditional PCM which often operate below freezing. Materials can optimize heating and cooling systems by providing on-demand thermal energy, although their efficiency is limited by cycle durability and temperature alignment.

To maximise the potential of electrification, decarbonising the electricity grid is integral. Countries like Norway, Bhutan, and Germany have made significant progress in reducing grid emission factors. India's grid emissions have already decreased from 850 to 700 grams per kWh, with targets set for further reductions.

Emerging Technologies

Thermochemical heat pumps, which utilise chemical reactions for heating and cooling, show great promise. These systems harness industrial waste heat, achieving high efficiency and significant decarbonisation potential. Similarly, desiccants, which separate moisture removal from cooling, offer substantial efficiency gains, particularly in humid regions.

The Path Forward

Decarbonising heating and cooling systems is critical for achieving global climate goals. This requires a multi-pronged approach. By integrating the above strategies, we can mitigate the environmental impact of heating and cooling while sustainably meeting growing global demand.

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DYNAMIC POWER PRICING IN ELECTRICITY MARKETS: DIGITAL ENERGY TRANSITION TOWARDS SUSTAINABILITY, SECURITY AND RELIABILITY

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Abstract:

Electrical power markets are undergoing a rapid transformation during the digital divide and energy transformation. There are many parameters which are assumed to be static, are changing dynamically. With continuous change in load and renewable generation, electricity load and price, which are strongly interdependent, forecasting of these parameters are challenging as they exhibit wide and varied volatility, which makes it difficult. The output of these parameters are used in a series of other programs which are used to compute and determine values which are used to help making decisions.

Smart Power Grids utilizing Information and Commutation Technology (ICT) accelerate the need for the targets towards net zero and de-carbonization. This paper attempts to address the issues of techniques and methodologies needed for realizing them. Real Time, Day Ahead, Balancing and Green Energy constitute a major part of Dynamic Electricity Markets that require complex computational calculations for determining various values like market clearing price (MCP), market clearing volume (MCV) required for electric energy trading. Power exchange for electricity markets uses digital trading methods over short durations. Application of Block chain based techniques for energy trading is the need of the hour for efficient dynamic pricing in electricity markets.

Dynamic Power pricing for energy transition towards green renewable energy for achieving net zero and de-carbonization is considered in this work. Energy internet and energy storage are gaining importance in the era of energy transition. Energy security, sustainability and reliability of power grids are strongly influenced by dynamic electric markets and parameters which are influenced by dynamic pricing. Case study of important applications using recent advanced technological methods are presented to validate the need for dynamic markets for energy transition towards net zero targets.

Keywords: Dynamic Markets, Electricity Pricing, Real time Day Ahead Markets,

Introduction:

Competition and Cooperation of electricity utilities are the basis of Deregulation and Restructuring of Generation Transmission and Distribution companies form vertically-integrated dependent monopolistic entities to horizontally-separated autonomous and independent ventures that encourage active private participation. The private participation in generation has led to competition in the supply of electricity from various vendors. This has led to variation in the prices of power generation in electricity markets, where generation companies (GENCOs) compete with each other to 'sell' or 'supply' power at a low price.

The distribution companies (DISCOs), also compete to 'buy' or 'purchase' power from the GENCOs. The various 'Buy' and 'Sell' offers introduces a 'variable' price of power in contrast to the fixed price. This variable price expressed in 'Rs. per MWh' has led to the development in 'trading in electricity markets'. This successful trading in electricity markets has been instrumental in developing various online trading platforms like PXIL, IEX, etc. Many more trading platforms have emerged leading to a vibrant and dynamic electricity markets for trading of power.

Single auction and double auction markets are emerged to determine the market clearing price 'MCP' and market clearing volume 'MCV' which leading to dynamic electric markets. Further, the variation in the generation and load has led to the variation in the electricity price. Forecasting of Generation, Load, Electricity Price, etc. play an important role in the operation of dynamic electricity

Real Time, Day Ahead, Balancing and Green Energy constitute a major part of Dynamic Electricity Markets that require complex computational calculations for determining various values like market clearing price (MCP), market clearing volume (MCV) required for electric energy trading. Power exchange for electricity markets uses digital trading methods over short durations

markets. Load Forecasting and Price Forecasting are important constituents that contribute to the development of Dynamic Electricity Markets.

Dynamic Electricity Markets (DEM), has further led to Dynamic Energy Markets which use advanced technological frameworks and policies in transition to energy sustainability. Dynamic Energy Markets provides a more open and challenging problem that encourages renewable energy resources and energy storage to participate in electricity markets. Based on the load demand, single auction and double auction markets are in use for effective competition ensuring dynamic electricity markets.

This paper addresses important issues which are related and effect the operation of Dynamic Electric and Energy Markets. Forecasting, Strategic Bidding, Auction Markets, Ancillary services, Pricing of Real and Reactive Power, etc.

Competition in dynamic electricity markets involves the interaction of the following four layers, namely, physical producers, financial traders, buyers and sellers. The competition of between the players is dependent on the volatility of electricity prices. Power generation from different types of producers like hydro thermal, pumped storage, etc.

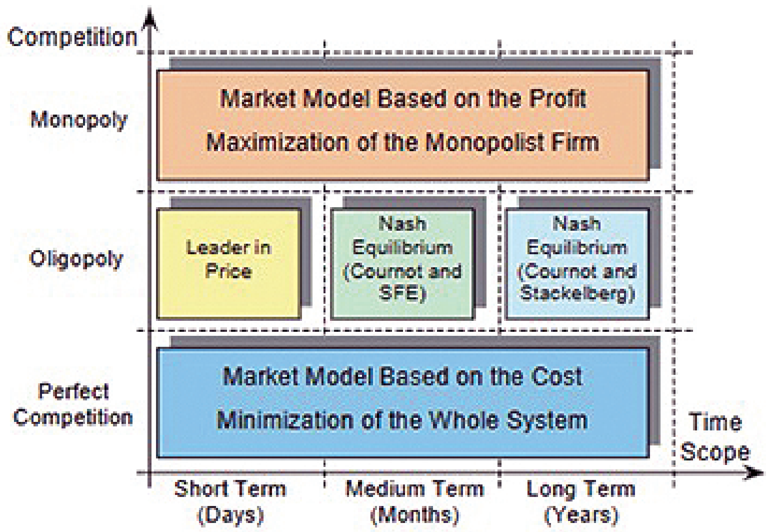


Fig. 1. Three types of electricity markets

Electric Markets

Electricity Markets consist of three important types, namely, Monopoly, Oligopoly and Perfect Competition. Fig 1 shows the three types of electricity markets

There are three types of electric markets

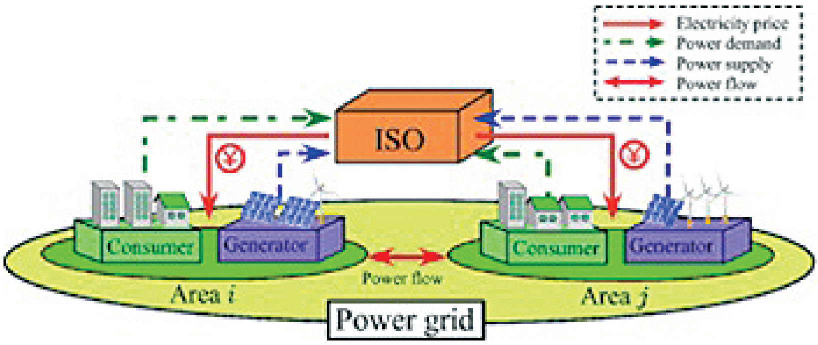
Monopoly electric market is a vertically integrated structure where all of the assets of generation, transmission, distribution, wholesale / retail sale of energy and operation functions are owned and operated as one entity

Oligopoly electric market consists of a few large utilities which dominate the selling of power with few substitutes for them. Oligopoly market structure restrict output or prices to achieve higher returns. The key characteristic of an oligopoly market is that not one of the firm can keep the others from having significant influence over the market. In this type of market each producer maximizes the profit

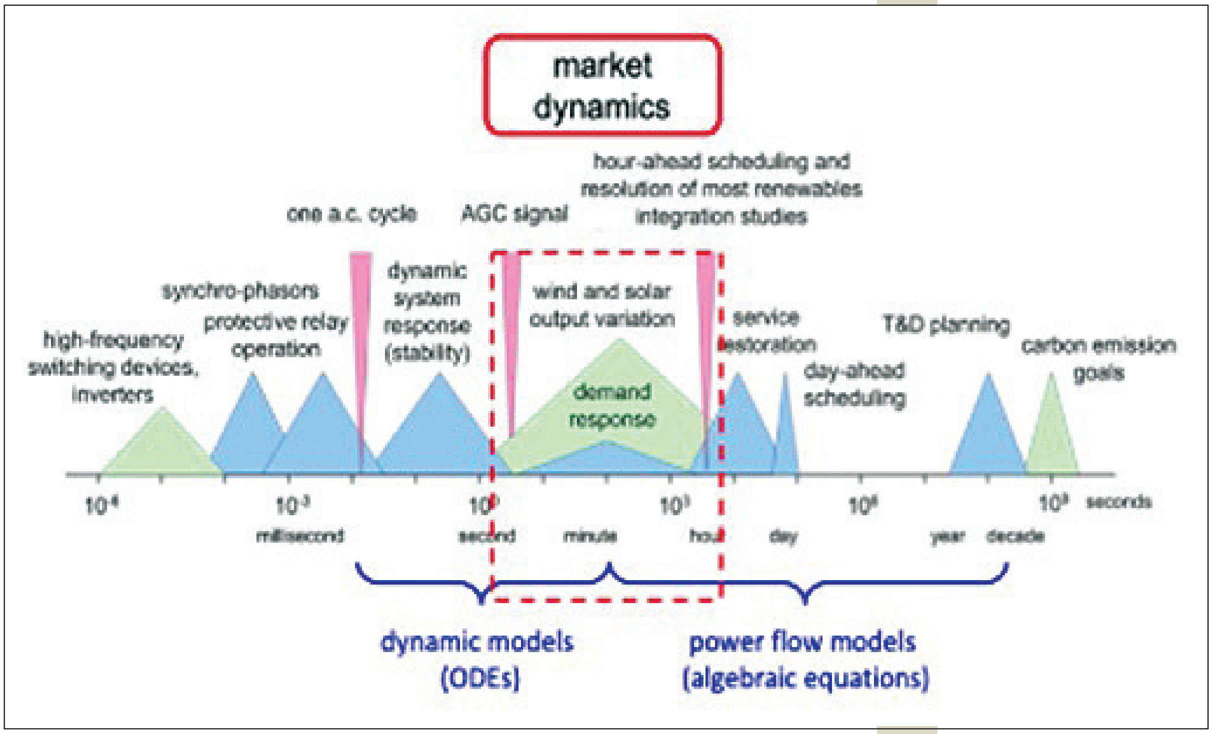
Perfect competition electric market consists of a price taking producer that wishes to maximize its profits by bidding his power production at his own marginal cost. Game theory plays an important role in competitive electricity markets.

Competition in dynamic electricity markets involves the interaction of the following four layers, namely, physical producers, financial traders, buyers and sellers. The competition of between the players is dependent on the volatility of electricity prices. Power generation from different types of producers like hydro thermal, pumped storage, etc. introduces uncertainty under competition in the operation and planning of dynamic electricity markets. Forward

Markets: The forward market schedules production a day in advance, and then a spot market that balances demand and supply immediately before operation. In such markets, generators have incentives to engage in intertemporal price discrimination. Forward markets are a type of electricity market that allow participants to lock in energy prices and quantities for the future. Forward markets can be medium-term or long-term.



(a) Dynamic Electricity Markets



(b) Market Dynamics

Fig. 2. Dynamic Electricity Markets and Market Dynamics

Dynamic Electricity Markets and Electricity Pricing

Dynamic electric markets consist of pricing in real time markets, where both generators and loads provide 'supply' and 'buy' bids in real time. Fig 2 shows the schematic of dynamic electric markets and market dynamics.

Dynamic pricing in real time markets is concerned with the delivery of electricity one hour before the closure of the market. Electricity Pricing and Volatility play an important role in the dynamic electric markets.

Electricity Pricing and Price Volatility

Forecasting of Electricity price is important aspect in the operation of Dynamic Electricity Markets. A common feature of restructured electricity markets is price volatility, due in large

The TV-PAR method will identify sources of volatility, capture short-term fluctuations, and understand how renewable energy impacts price stability. TVP-VAR model is a statistical tool that can capture the changing nature of economic relationships over time

part to the difficulty in storing electricity for the purpose of smoothing price fluctuations. Price volatility is a common feature in deregulated wholesale electricity markets which is a consequence of inelastic demand and power generation.

Real Time Pricing:

Real time pricing (RTP) is a model that adjusts process in response to market changes of supply and demand. RTP, also known as dynamic pricing, is used to adjust the price of electricity based on the current supply and demand. RTP is concerned with changes involved in the electricity price in small intervals based on the market conditions. RTP plays an important role in smart grid infrastructure. Dynamic pricing involves making adjustments to the electricity price in real time under market dynamics. Real-time pricing (RTP) tariffs are charged over very small intervals to reflect the true nature of fluctuating energy prices. RTP reflects the utility's production cost in real time to supply the consume with various choices for different applications like EV charging, residential applications, etc.

Time-Varying Parameter Vector Auto Regression (TVP-VAR) Method

Time-Varying Parameter Vector Auto Regression (TVP-VAR) is a method is used for the addressing the price volatility in dynamic energy markets. The TV-PAR method will identify sources of volatility, capture short-term fluctuations, and understand how renewable energy impacts price stability. TVP-VAR model is a statistical tool that can capture the changing nature of economic relationships over time. It's used to analyze macroeconomic issues and other areas where parameters may change over time. TVP-VAR forecasts economic variables and analyze structural changes in time series, which is used to predict price changes. TVP-VAR models can be used to study the relationship between price and other economic variables in the electric market. These models can capture how the relationship between variables changes over time. TVP-VAR models are a type of time series model that explain how economic variables change over time. They model the coefficients of the model as stochastic processes, such as random walks.

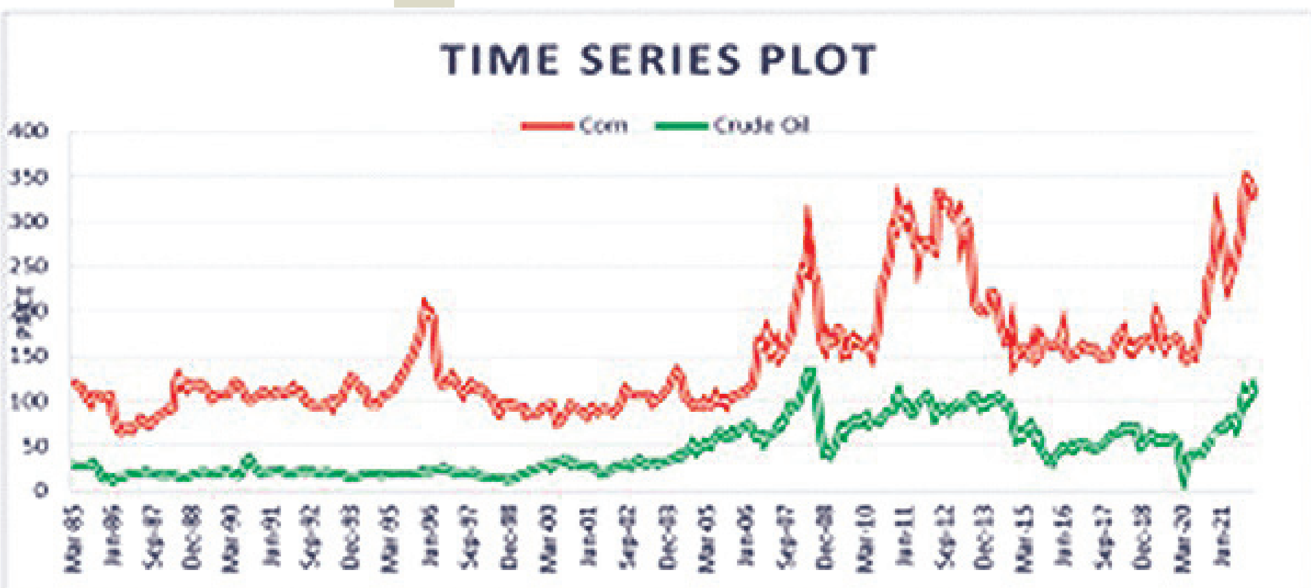


Fig. 3. Time series plot of varying electrical prices with fuel (crude oil) using TVPVAR

Figure 3 shows the typical timeseries plot of electrical prices with fuel using TVPVAR

Load and Price Forecasting

Load Forecasting

Linear regression and Neural Network models are used to forecast the demand. The results of the above models are compared and the better model is retained. The relation between day-ahead price and the old values of price is studied using autocorrelation. Using the forecasted load and externally obtained temperature and fuel cost data the price is forecasted using a modified Neural Network. In many countries, the power industry is moving towards a competitive framework, replacing the highly regulated procedures. The main objective of an electricity market is to decrease the cost of electricity through competition. Competition results in an efficient utilization of resources. The electrical energy cannot be appreciably stored, and the power system stability requires constant balance between supply and demand. Load serving bodies will get to know the amount of power consumers are likely to use and the ways of securing it cheaply. Large industries will schedule their schedulable loads based on the variation of price with time. The companies that trade in electricity markets make extensive use of price prediction techniques either to bid or to hedge against volatility.

Stochastic models like Auto Regression, Moving Average, Auto Regressive Moving Average are stationary processes – they work well if the error distribution has a mean equal to zero and variance constant. So, we cannot use them to forecast the price of electricity (Mean Average Percentage Error varies from 4% to 10%), Linear regression models can only forecast the week average prices whereas non-linear regression models demand us to assign exact non-linear function for better forecasts

Load forecasting – Inputs

The following inputs are considered for demand forecasting

1. Temperature (maximum temperature of the day in oC)

2. Hour of day

3. Day of the week

4. A flag indicating if it is a holiday/weekend

5. Previous day's average load (in MWh)

6. Load from same hour the previous day

7. Load from same hour and same day from previous week

Load forecasting – Case Study

The day-ahead demand is forecasted using Linear regression and Neural Networks. Data of many parameters like hourly temperature, demand, electricity price and fuel costs were obtained for a period of four years for the residential area of New England ISO market from www.iso-ne.com. The system is trained using the data for years 2004 – 2007 and the model is then tested for the year 2008

Linear Regression:

The output is assumed to be linearly dependent on the inputs

$y = \beta_0 + \beta_{1x1} + \beta_{2x2} + \beta_{3x3} + \ldots + \beta_{kxk} + e$

β_is are the regression coefficients that are found by the least square error method. Least square function (L) for 'n' observations is

$L = \sum ni=1(yi - \beta_0 - \sum kj=1 \beta_j x_{ij})2$

3. The above equation on differentiating with respect to β_0 and β_js will give k+1 linear equations and all β_s can be found

The load data for 2008 is compared with predicted data obtained from the model to ascertain the accuracy of the model

The accuracy is statistically determined using the Mean Absolute Percentage Error (MAPE) as the metric

MAPE is defined as :

MAPE (%) = {100 ∑ni=1 | (Actuali - Forecasti) / Actuali | }/n

In many countries, the power industry is moving towards a competitive framework, replacing the highly regulated procedures. The main objective of an electricity market is to decrease the cost of electricity through competition

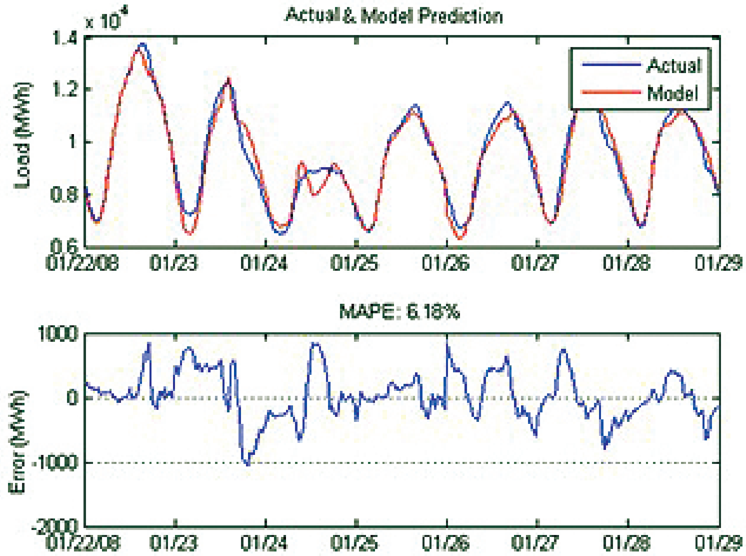


Fig. 4. Load Forecasting and error in Forecasting

A two-layer feed forward network with demand as the sole output is used to forecast the demand. The weights generally get assigned such that an input with small values will have larger weights compared to inputs with large values

Figure 4 shows the plot comparing the demand available in the data with that predicted by the model (LR) along with the MAPE. As can be seen in the plot the peaks are not properly captured as they are non-linearly dependent. MAPE of 6% for demand forecast is not good. Hence, Neural network is used. The Mean Absolute Percentage Error of the forecasted load throughout the year 2008 using Linear Regression is as shown below.

Load Forecasting using Neural Networks:

A two-layer feed forward network with demand as the sole output is used to forecast the demand. The weights generally get assigned such that an input with small values will have larger weights compared to inputs with large values. So, the inputs are all initially normalized to the range [0,1] so that the system is not confused with different scales of weights, using the relation Scaled_x = (x – xmin)/(xmax – xmin)

The fully connected neural network is initially assigned random weights and biases between -0.5 and 0.5. The scaled inputs are fed into the network and the output 'yo' is obtained which is compared with desired output 'do'. The output error is defined as

erroro = yo(1- yo)(do - yo)

Now, using the back propagation algorithm weights(w) and biases(Θ) corresponding to the path from the hidden layer to output layer are updated and then the weights in the path from input to hidden layer are updated

Δwij = l.errorj.oi; w'ij = wij + Δwij ; ΔΘj = l.errorj

where, l is the learning rate and l = 1/k where k is the number of iterations performed by the network

Figure 5 shows the load forecasting using ANN. The input is fed into the updated neural network and the process is continued until one of the following conditions are achieved. The Δwij of all the paths are below a minimum value (0.01). The total number of cycles of training completed is more than a maximum value (60000). The trained neural network is now used to predict the load of year 2008 and the model data is compared to the actual data

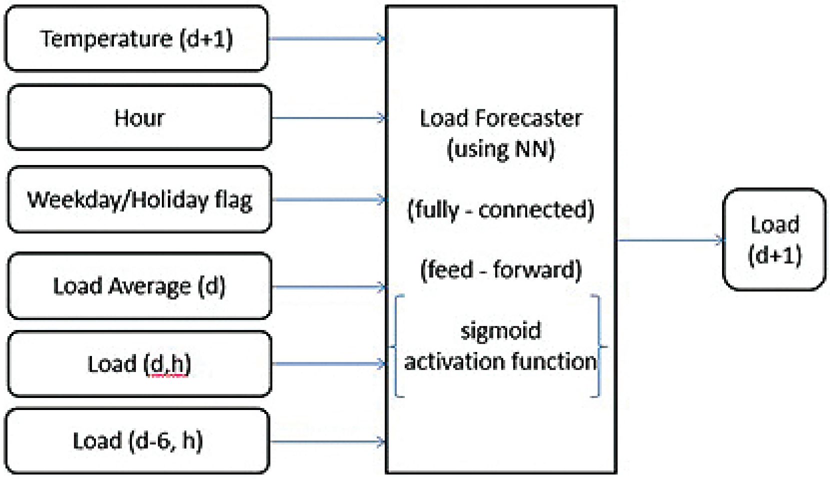


Fig. 5. Load Forecasting using Artifical Neural Networks

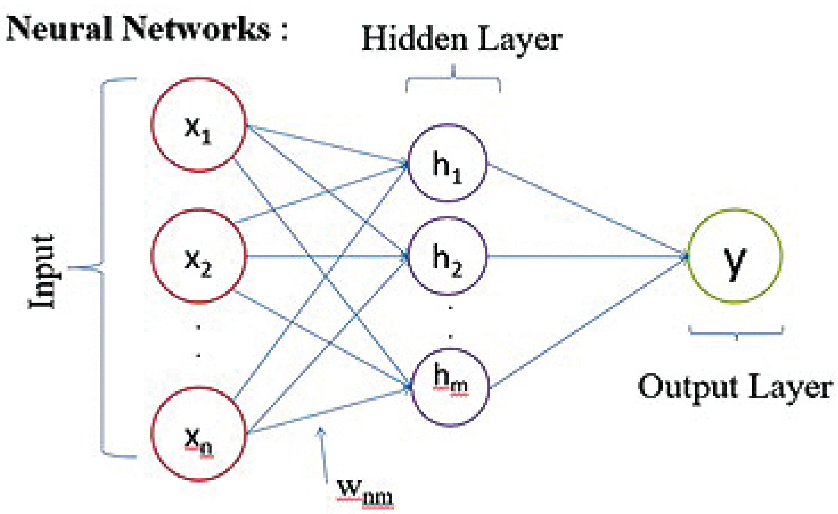


Fig. 6. Artifical Neural Network architecture for Load Forecasting

Figure 6 shows the ANN approach to load forecasting.

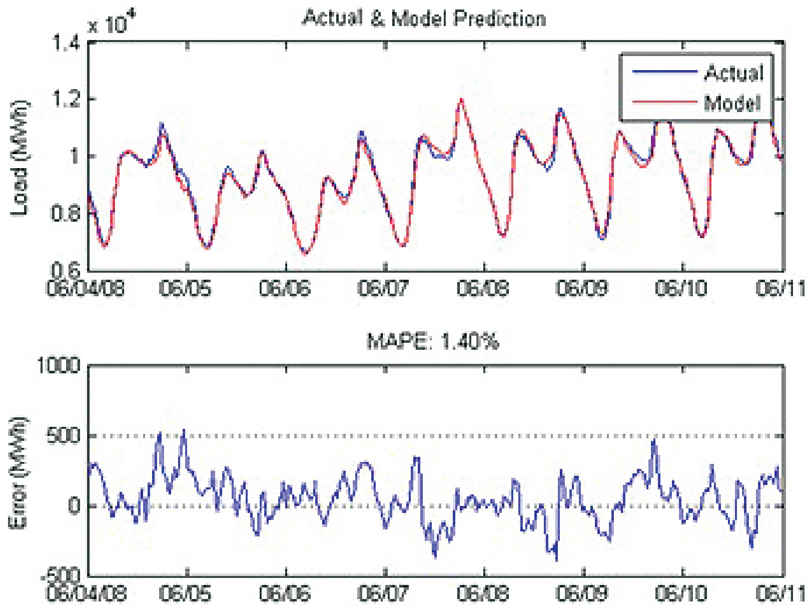


Fig. 7. ANN approach to Load Forecasting and error

The input is fed into the updated neural network and the process is continued until one of the following conditions are achieved

A plot comparing the demand available in the data with that predicted by the model (NN) along with the MAPE is shown in figure 7. As can be seen in the plot the peaks are also properly captured. MAPE of 1.4% for demand forecast is a very good forecast. The MAPEs of the forecasted loads throughout the year 2008 was found to be 6.4% for the Linear Regression model and 1.78% for the Neural Network model. Hence, Neural Network model is preferred over Linear Regression model to predict the demand in the market

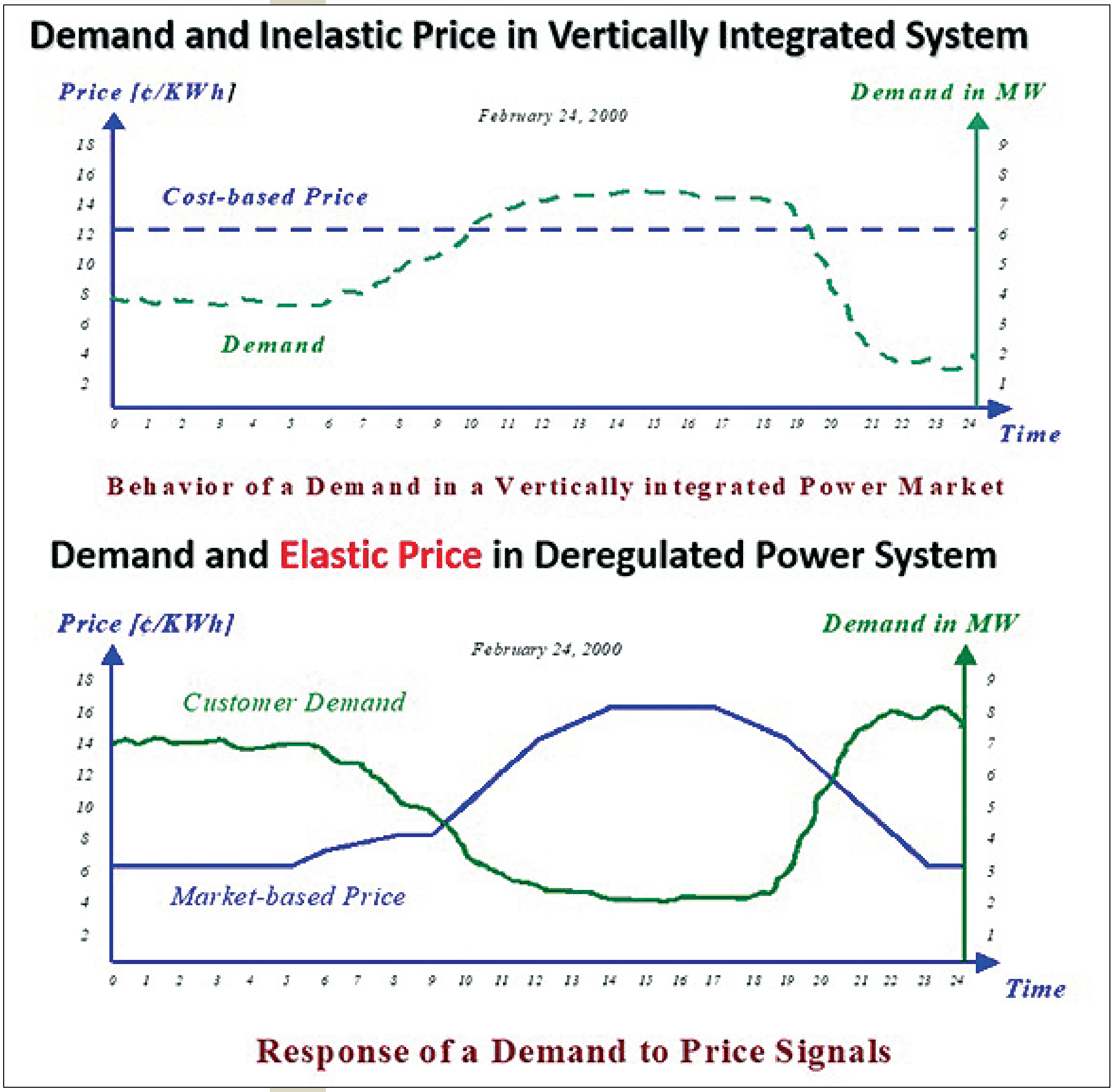


Fig.8. The dependance of Electricity Price on Load and its price and volatility.

The following inputs are considered to forecast the price of electricity:
1. Temperature (0C)
2. Hour of day
3. Day of the week
4. A flag indicating if it is a holiday/weekend (binary)
5. Forecasted load (MWh)
6. Previous day's average load (MWh)
7. Load from the same hour the previous day (MWh)
8. Load from the same hour and same day from the previous week (MWh)
9. Previous day's average price ($/MWh)
10. Price from the same hour the previous day
11. Price from the same hour and same day from the previous week
12. Previous day's fuel price (S/litre)
13. Previous week's average fuel price

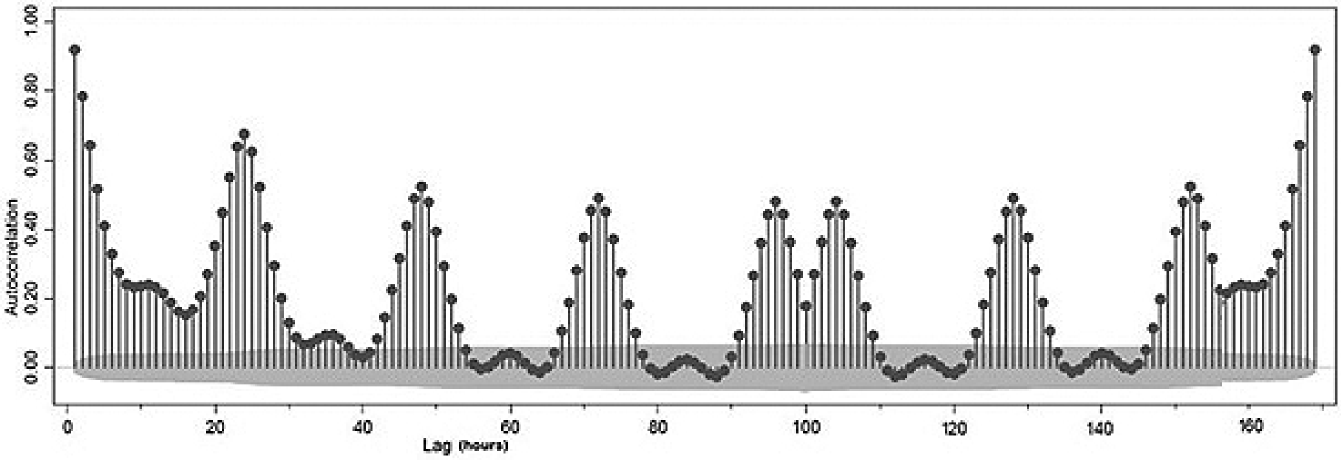


Fig. 9. Autocorrelation of electricity price

Figure 9 shows the Autocorrelation of electricity price obtained as explained above.

Price Forecasting using ANN

The price is significantly correlated with 24-hour earlier price and keeps reducing for the previous days. The price is more significantly correlated with 168-hour earlier price (7 days). Although the auto-correlation with respect to previous hour price is as high as 0.9, the data cannot be used as input since it is not available at the time of forecasting. Hence, previous day same hour price and previous week same hour prices are considered to forecast the price. The neural network is initially run in the normal manner and the weights and biases are stored. The Mean Square Error of the whole samples that were used to train the network is calculated. The MSE is now added to the output and this is considered as the new output. The training is continued with the new output and the stored weights.T he MAPEs of the two iterations are compared and the algorithm continues until new MAPE is less than the old. Apart from the MSE method, the problem of over-fitting and local minima are addressed. Over-fitting is the inability of the network to perform on the test data despite working well while training.

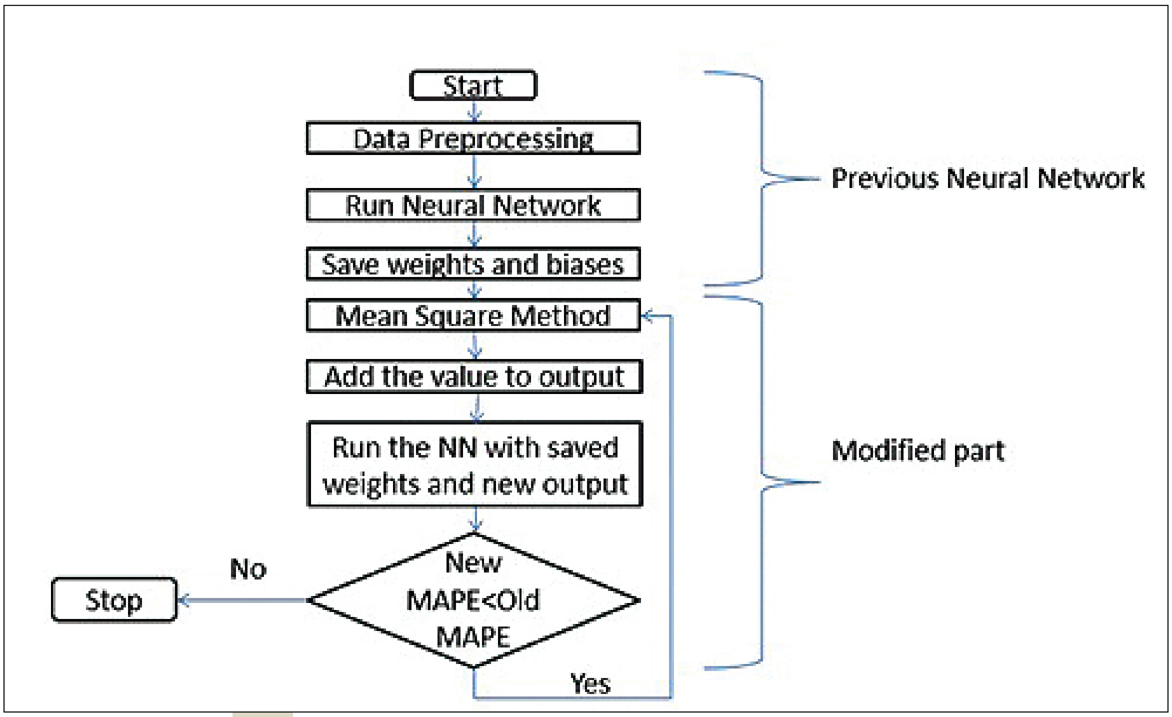


Fig 10. Price Forecasting using neural Networks

Figure 10 shows the ANN approach to price forecasting.

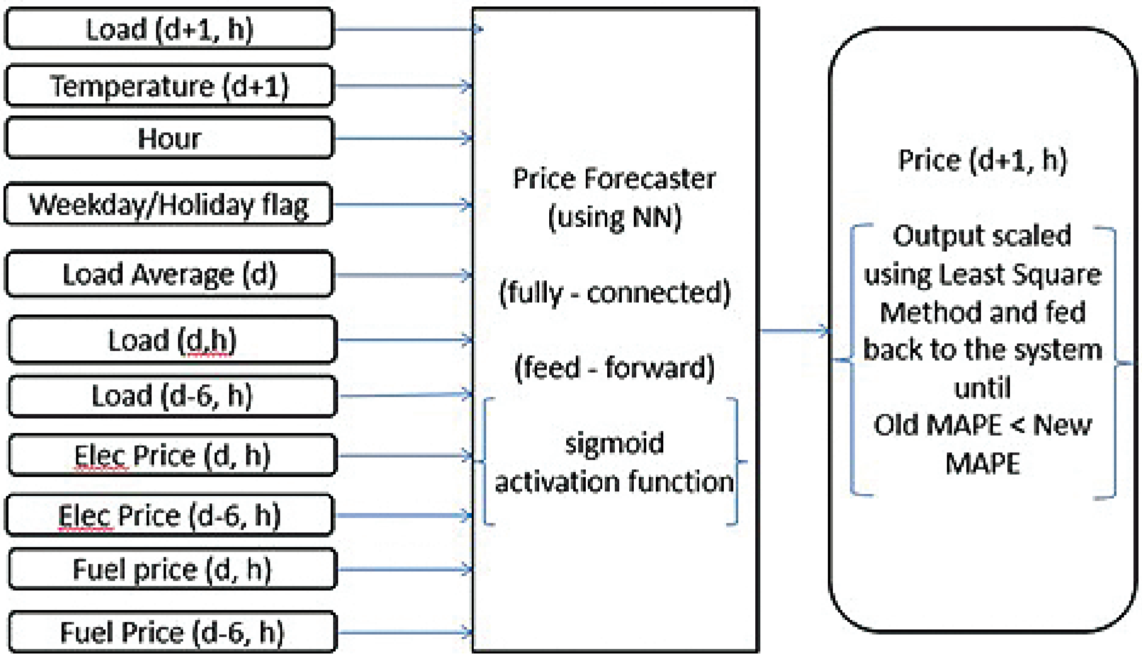


Fig 11. Architecture of Price Forecasting using neural Networks

Figure 11 shows the architecture of price forecasting using neural networks.

The same data that was used in the earlier case study to forecast the load is used to forecast the price. The model is trained using data from 2007 – 2008 and forecasted for the year 2008. The forecasted price is compared with the actual price for the whole year. The correctness of the model is determined using the statistical metric MAPE

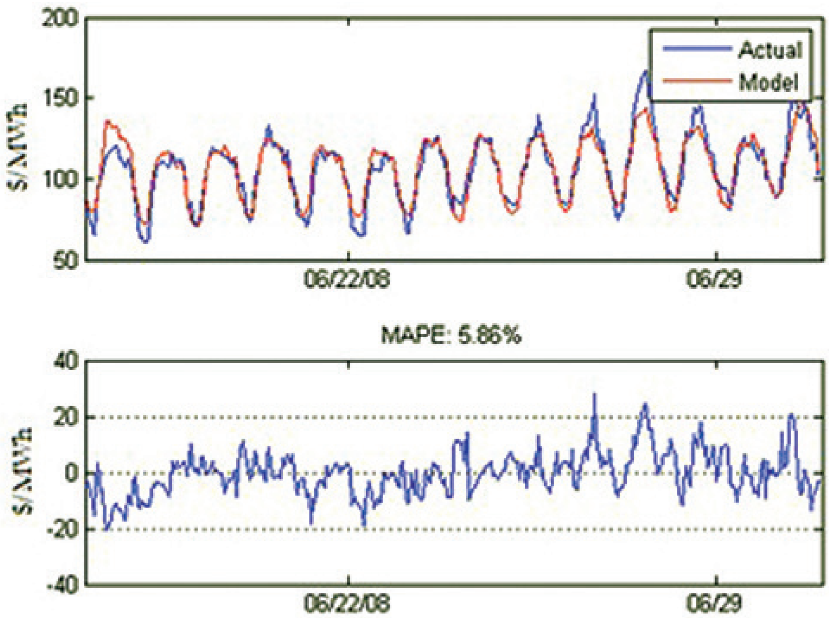
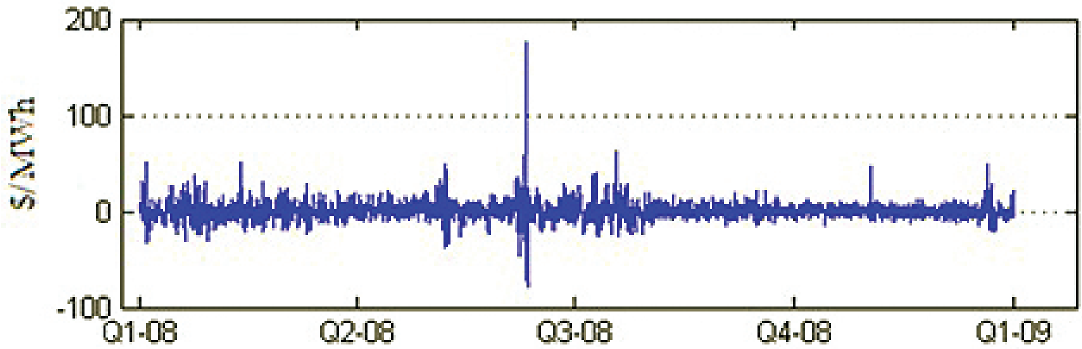


Fig 12. ANN Approach to Electricity Price Forecasting

Figure 12 shows the results of ANN approach to price forecasting.

Price forecasting – Case Study

The error is acceptable throughout the year but during the months of May and June the error is high because of the fluctuating demand. The Mean Absolute Percentage Error of the forecasted price is as shown in figure 13.



TRANSMISSION PRICING IN DYNAMIC ENERGY MARKETS

Dynamic Energy Market consist mainly of electricity pricing from generation to generation through transmission. There are many transmission pricing schemes. This consists of the following

Evaluation of the various embedded cost transmission pricing schemes. Social Welfare Maximization (i.e., in case of constant load it is minimization of total generation cost). Calculation of the nodal pricing and Congestion management studies. Transfer capability evaluation in deregulated environment. Evaluation of transmission pricing such as Embedded cost pricing and Incremental cost pricing. Embedded cost is evaluated using the postage stamp method and MW-mile method and Incremental cost is evaluated using (SRMC) method. Congestion management studies have been carried out by imposing restrictions on the transmission capacity of the lines and considering severe contingencies. Available Transfer Capacity calculations have been done considering different contingencies including bilateral and multilateral transactions.

Evaluation of Embedded Cost Pricing for an 8-bus network. Congestion management Studies, Calculation of Nodal pricing and Transfer Capability Calculations in Deregulated Markets for 11-zone DC network and 23- Bus AC network

Open Transmission Access (OTA): Requirement That the Transmission Network Owners make Their Systems Available to Other Players In The System.

Independent System Operator (ISO): Supreme entity to control the transmission system which is responsible for secure system operation and to maintain system reliability.

Schedule Coordinator(SC) / Broker: Match electric energy supply and demand based on bid prices

Bilateral Transactions: suppliers and consumers independently arrange trades without causing any limit violations under postulated contingencies, the system is judged to be capable of accommodating these transactions

Multilateral Transactions: It is a trade that is arranged by energy brokers and involves more than two parties.

ongestion: Condition where demand for power transmission exceeds system's capability

encos: Operates and maintains generating plant

Discos and Retailers

Discos maintains the distribution network and provides facilities for electricity delivery. Retailers provide electric energy sales to end consumers.

Evaluation of the various embedded cost transmission pricing schemes. Social Welfare Maximization (i.e., in case of constant load it is minimization of total generation cost). Calculation of the nodal pricing and Congestion management studies

TRANSMISSION PRICING METHODS

Embedded Cost

Transmission Pricing consists of two methods like Postage stamp method and MW-Mile method. Incremental Cost Transmission Pricing consists of two methods like Short Run Marginal Cost Pricing (SRMC) and Long Run Marginal Cost Pricing (LRMC)

Embedded Cost Pricing

Postage Stamp Method is a simple method where the transmission charges based on weight of the package magnitude of transaction power. It is charged at a flat rate on per MW basis where short distance customers may bypass the system due to high transmission prices

$R_t = TC * P_t / P\ peak$

where, R_t - transmission price for transaction t in Rs

TC – total transmission charges in Rs

P_t - load at time of system peak load condition in MW

P_{peak} -system peak load in MW

MW-Mile Method:

The transmission network capacity use for firm transmission services including wheeling transactions, by including the path and distance traveled by the wheeled power. There is no dispute over order of wheeling transaction. It mitigates the threat of uneconomical transmission bypass by providing better cost signals to both long and short distance wheeling customers

$R_{Ti} = [\, Pj;Ti * Lj * Fj / (P_j;T_i)\,]$

R_{Ti} - price charged for transaction Ti

$P_j;T_i$ – loading of line j due to transaction Ti

L_j – length of the line j

F_j – pre-determined unit cost reflecting the cost per unit capacity of line

Incremental Cost Pricing

This pricing method seeks to identify the additional burden on a transmission system from one particular transaction

1. Short-Run Marginal Cost (SRMC) pricing: where the cost incurred in supplying an additional 1MW of power in a transaction (for operation decisions)

2.Long-Run Marginal Cost (LRMC) pricing: In this long term planning analysis and network upgrades included within the transactions (for investment and location decisions) which includes new transmission line addition and power transactions brought about for these additions.

Various methods to evaluate Transmission Network Capacity use for firm transmission services including wheeling transactions. MW-Mile method is more reflective of the actual usage of transmission network in allocating the transmission network capacity cost than postage stamp method. The potentials for realizing greater economic efficiencies through use of MW- mile method.

OPF BASED PRICE CALCLATION

OPF BASED PRICE CALCLATION

$$MaxF = \left(\sum_{j=1}^{n} Bj(Dj) - \sum_{i=1}^{n} Ci(Gi)\right)$$

Problem formulation for Social Welfare Maximization is

$$\left(\sum_{j} D_j - \sum_{i} G_i + L\right) = 0$$

Subjected to

$$(G_i - G_{i,max}) \le 0 \quad : \forall\, i$$
$$Z_k \le 0 \quad : \forall j$$

where i and j are the set of producers and purchasers, G and D their respective generation and consumption and producer offer (bid) price and purchaser benefit (utility) functions are given by C and B respectively

L is a transmission loss function,

$G_{i,max}$ generator i capacity and

Various methods to evaluate Transmission Network Capacity use for firm transmission services including wheeling transactions. MW–Mile method is more reflective of the actual usage of transmission network in allocating the transmission network capacity cost than postage stamp method

Z_k the k^{th} operating constraint

In case of price inelastic load, the objective is to minimize total generation cost subject to all relevant constraints

$$\underset{G_i}{Min} \sum_{i} C_i\,(\,G_i\,)$$

•Equality constraints
-bus real and reactive power balance
-generator voltage set points
•Inequality constraints
-transmission line/interface flow limits
-generator MW and MVAR limits
-bus voltage magnitudes

Tranactive Energy Markets

Transactive Energy is a system of economic and control mechanisms that allows the dynamic balance of supply and demand under various scenarios. The trans-active energy approach offers a way for producers and consumers to more closely match and balance energy supply and energy demand. Trans-active Energy Market (TEM) allows consumers and utility companies to trade energy, which can improve the efficiency and reliability of the power grid. TEM framework is proposed to enable and incentivize DER owners, including Wind Power Generation (WPG) and Hydrogen Energy Storage (HES) to participate in Day Ahead and Real time markets. The Transactive Energy Market (TEM) approach for energy management and trading, facilitates the integration and participation of distributed energy resources (DERs) in existing networks using market-based solutions for energy management. Trans-active Energy Management is type of active energy management optimization framework which examines all flexible loads and generations using bidirectional communication for information exchange for the of end-use DERs.

The Transactive energy management approach allows both the demand and supply to actively negotiate the exchange of energy. Transactive energy, employs the Grid Wise Architecture Council (GWAC), which uses both economic and control methods that model the dynamic balance of supply and demand across the entire electrical network. Transactive energy encourages dynamic demand-side energy activities based on economic incentives and ensures that the economic signals are in line with operational goals to ensure system reliability without resorting to override control. In transactive energy management, decision making is transferred to DERs. Through a distributed decision-making process, all DERs are able to decide on their actions in energy management, without revealing their private information.

Transactive energy markets offers key benefits to consumers. Better utilization of grid assets can lower costs, especially during peak demand conditions. Greater resilience and reliability in large storms will reduce the length and frequency of outages. Increased choice and information will give consumers greater control over personal energy use. Increased use of renewable energy resources will give individual consumers the satisfaction of contributing to larger, societal environmental goals.

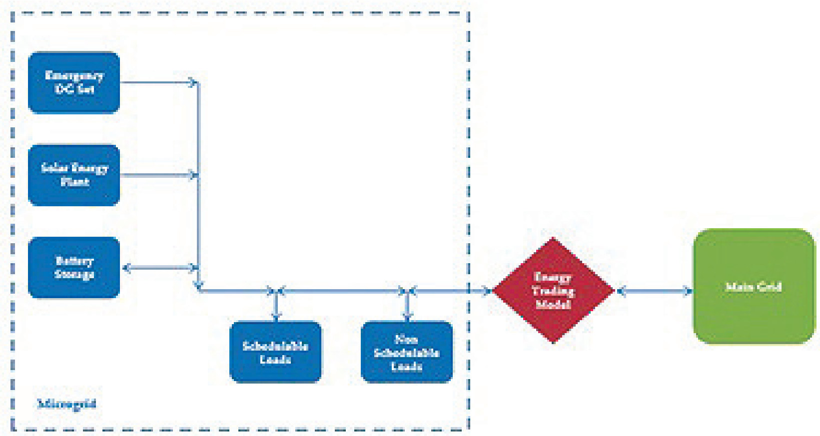
In dynamic electricity markets, transactive energy approach has many benefits to customers in terms of customer response when the grid is overloaded. By providing tools to the customers to manage and adjust timing of energy usage for reducing the fluctuations in energy through “demand response”. Increased use of cost-effective, renewable energy generation (especially from variable sources like wind and solar) will require new tools for operating the grid, and TE can provide these tools. Transactive energy enables the enhancement of the reliability and resilience through dynamic pricing. Market Dynamics incentivize grid-responsive technologies and grid-friendly consumer behavior

Transactive energy markets offers key benefits to consumers. Better utilization of grid assets can lower costs, especially during peak demand conditions. Greater resilience and reliability in large storms will reduce the length and frequency of outages. Increased choice and information will give consumers greater control over personal energy use

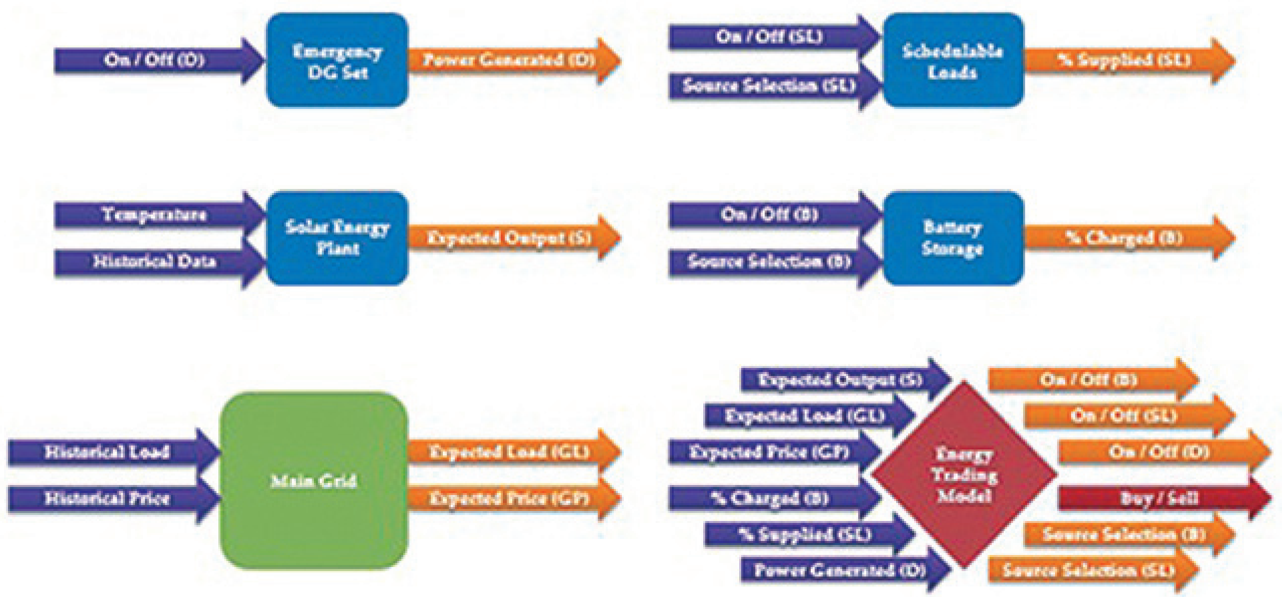
which help in efficiency and reliability.

Dynamic Pricing Markets of Micro Grid Energy Trading

A Microgrid Energy Trading Model incorporating dynamic pricing is developed which is based on energy economics which is expected to make profitable trading decisions. The model takes all the constraints in the system in to consideration. Figure 14. below show the working of the Dynamic Micro Grid Energy Trading for Profitable Scheduling



(a) Architecture of micro grid model



(b) Individual models of the microgrid

Fig. 14. Microgrid Architecture Model for Dynamic Energy Trading

Description of the modules: Building a system to perform the following tasks of i) forecasting Solar Energy production in the Microgrid, ii) forecasting the electricity price in the deregulated markets and iii) Profitable scheduling of the loads in the Microgrid selected

The problem is considered as three parts

Part A: Forecasting: To forecast electrical price and demand in a deregulated market and Solar Energy generation in the smart grid based on historical data

Part B: Scheduling: To build a model capable of making profitable decisions using the forecasted values in Part A

Part C: Risk Analysis:

Evaluate the risk due to error in forecasting

Solar Energy Forecast = Solar Irradiation x Efficiency(η)

Efficiency (η) can be obtained from the manufacturer

Input parameters for forecasting Solar Irradiation using linear regression:

Historical Data (Y)

Temperature of the day (X)

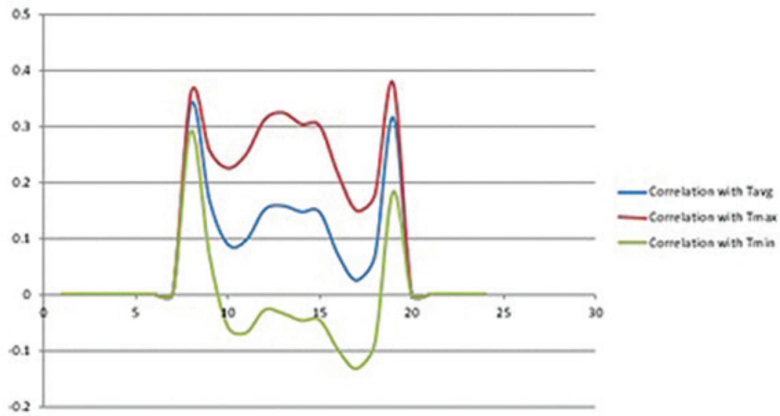
$$Forecast = a + bx$$

$$a = \bar{y} - a\bar{x}$$

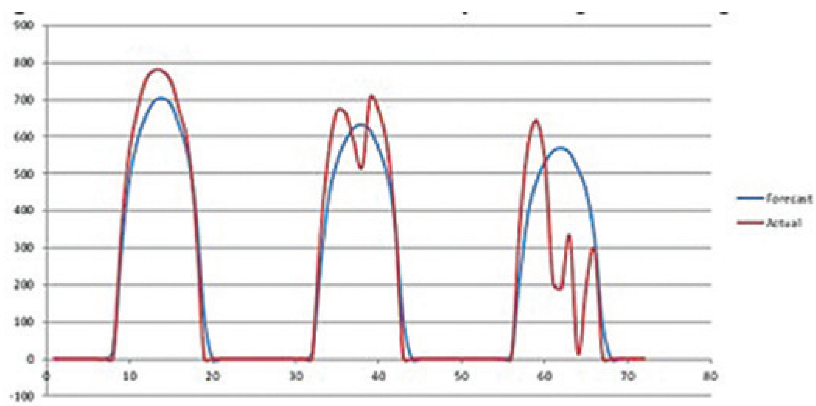
$$b = \frac{\sum(x-\bar{x})(y-\bar{y})}{\sum(x-\bar{x})^2}$$

Figure 15 shows the linear regression approach to Forecasting of Solar Irradiation and its dependence with temperature

An important input to the decision-making activities of a GENCO is a good forecast of the market prices. This is important because an accurate forecast of the short-term market price helps the GENCO to bid for power sell or buy appropriately and strategically, thereby providing higher returns



(a) Solar Irradiation plot



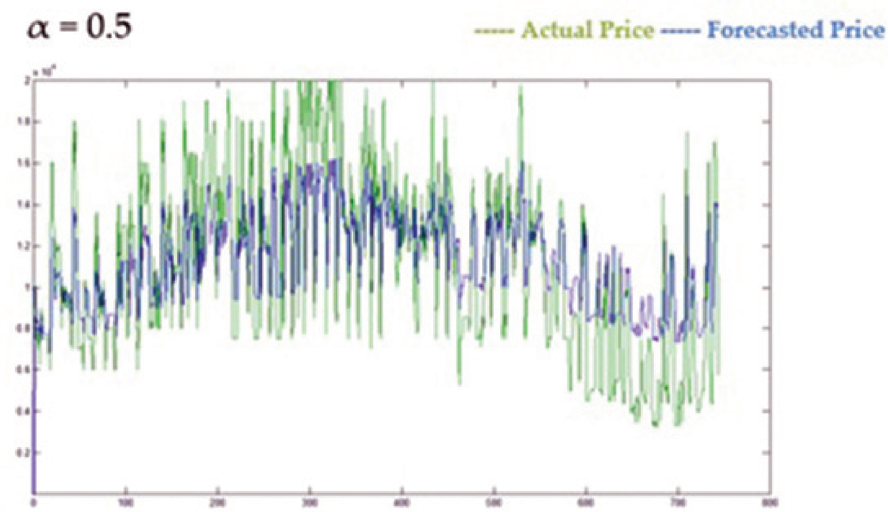
(b) Actual Forecasted Value of Solar Irradiation

Forecasting using Maximum temperature of the day as input and Historical data (2500 days) using linear regression

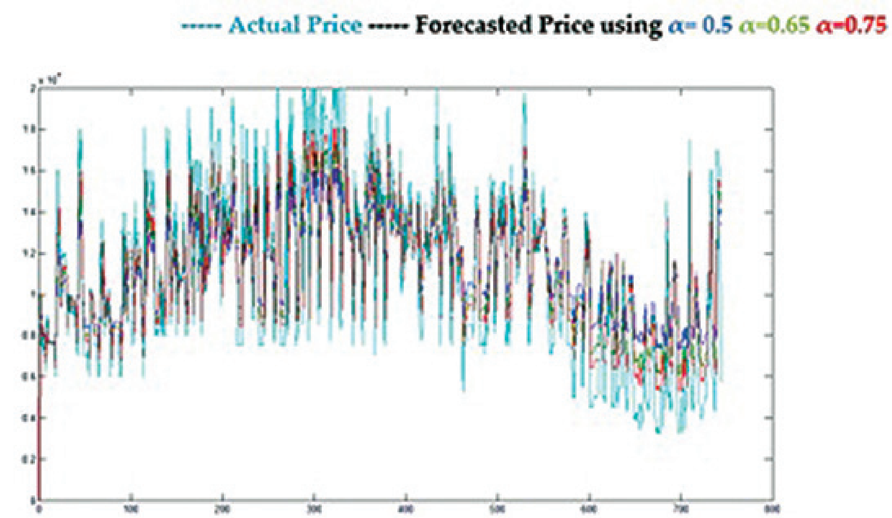
Forecasting Electricity Price (Rs/kWh) using MA model is shown by the relation

Price(n+1) = Price(n) + α* {Rate(n) - Moving Average(n)}

The results of forecasting for different values of α= 0.5, 0.65 and 0.75 are shown in fig 16.



(a) Price Forecasting



(b) Price Forecasting with different parameters

Electricity price forecasting is an important component energy trading in dynamic electricity markets.

Market Price Forecast

An important input to the decision-making activities of a GENCO is a good forecast of the market prices. This is important because an accurate forecast of the short-term market price helps the GENCO to bid for power sell or buy appropriately and strategically, thereby providing higher returns. Bilateral contract prices also have a tendency to be indirectly affected by spot-price trends. Thus good spot market price forecasts can help set up profitable bilateral contracts. In the short-term markets, continuous trading up to two hours in advance of real time is possible. In these markets, the prices can be highly volatile to system conditions such as sudden outages, and external factors such as temperature variations, rainfall, etc. It is usually of great interest to GENCOs and other market players to have a good forecast toolbox for these prices. Price forecast in the general sense also include forecast of futures and forward market prices. These forecasts may be carried out months or even a year in advance. These forecasts may be useful if the GENCO is contemplating investments in generation capacity, market risk analysis, production and maintenance planning, among others.

Price forecast in the general sense also include forecast of futures and forward market prices. These forecasts may be carried out months or even a year in advance. These forecasts may be useful if the GENCO is contemplating investments in generation capacity, market risk analysis, production and maintenance planning, among others

In a power market, the price of electricity is the most important signal to all market participants and the most basic pricing concept is market-clearing price (MCP). Generally, when there is no transmission congestion, MCP is the only price for the entire system. However, when there is congestion, the zonal market clearing price (ZMCP) or the Locational Marginal Price (LMP) could be employed. ZMCP may be different for various zones, but it is the same within a zone. LMP can be different for different buses. Figure 17 shows the power purchase in energy brokerage system.

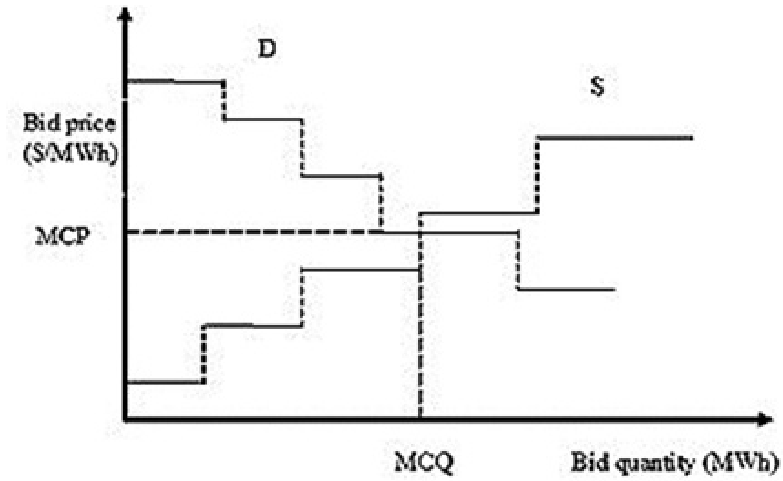


Fig.17. Power Purchase and Sell Bids in Energy Brokerage System

LMP is the cost of supplying the next MW of load at a specific location, after considering the generation marginal cost, cost of transmission congestion, and losses

MCP Calculation:
After receiving bids, ISO aggregates the supply bids into a supply curve (S) and aggregates the demand bids into a demand curve (D). In Figure 17, the intersection of (S) and (D) is the MCP.

ZMCP Calculation:
If at a given period, the ISO detects congestion along any transmission paths, it will adjust its zonal schedules at the two ends of each path to relieve the congestion. Accordingly, the MCPs in the two regions could be different which are denoted as zonal MCP (or ZMCP). Using ZMCP, we calculate the congestion charge (or usage charge) for each congested transmission path across that path.

LMP Calculation:
LMP is the cost of supplying the next MW of load at a specific location, after considering the generation marginal cost, cost of transmission congestion, and losses. That is, LMP is the sum of generation marginal cost, transmission congestion cost, and cost of marginal losses, although the cost of losses is usually ignored. When there is no congestion, LMP is the same as MCP. When there is congestion, the optimal power flow (OPF) solution considers transmission line constraints in order to balance supply and demand at each bus. The marginal cost of each bus is the LMP.

Electricity Price Volatility

The most distinct property of electricity is its volatility. Volatility is the measure of change in the price of electricity over a given period of time. It is often expressed as a percentage and computed as the annualized standard deviation of percentage change in the daily price (other prices such as weekly or monthly prices can also be used), Compared with load, the price of electricity in a restructured power market is much more volatile. From the curves, we learn that:

The load curve is relatively homogeneous and its variations are cyclic.

The price curve is non-homogeneous and its variations show a little cyclic property.

Although electricity price is very volatile, it is not regarded as random. Hence, it is possible to identify certain patterns and rules pertaining to market volatility. For example, transmission congestion usually incurs a price spike which is not sustained as electricity price would revert to a more reasonable level (this is known as mean reversion in statistics). It is conceivable to use historical prices to forecast electricity prices. Accordingly, we use a training scheme to capture perceived patterns for forecasting electricity prices. The fundamental reason for electricity price volatility is that the supply and demand must be matched on a second-by-second basis as follows, namely, Volatility in fuel price, Load uncertainty, Generation uncertainty (outages), Transmission Congestion, Behavior of market participant (based on anticipated price), Market manipulation (market power, counterparty risk)

Because of the special properties of electricity, the price of electricity is far more volatile than that of other relatively volatile commodities. The annualized volatility of oil future contracts is around 30%; it is around 50% for natural gas future contracts, while about 60% for electricity future contracts. In electricity spot markets, annualized volatility is above 200%. Because of the significant volatility, it is difficult to make an accurate forecast for the spot market of electricity. This is evidenced by the fact that the existing price forecasting accuracy is far lower than that of load forecasting. However, price forecasting accuracy is not as stringent as that of load forecasting.

Need of Price forecasting

The power awarded to each bidder is determined based on the individual bid curves and the MCP. All the power awards will be compensated at the MCP. After the auction closes, each bidder aggregates all its power awards as its system demand, and performs a traditional unit commitment or hydrothermal scheduling to meet its obligations at minimum cost over the bidding horizon. Suppliers' bidding decisions are coupled with generation scheduling since generator characteristics and how they will be used to meet the accepted bids in the future have to be considered before bids are submitted. Therefore, bidding decision must consider the anticipated MCP, generation award and costs, and competitor's decisions. The MCP and MCQ (market clearing quantity) are the most important power market indicators. Forecasting the hourly MCP and MCQ in daily power markets is the most essential task and basis for any decision making in the power market.

The fundamental reason for electricity price volatility is that the supply and demand must be matched on a second-by-second basis as follows, namely, Volatility in fuel price, Load uncertainty, Generation uncertainty (outages), Transmission Congestion, Behavior of market participant (based on anticipated price), Market manipulation (market power, counterparty risk)

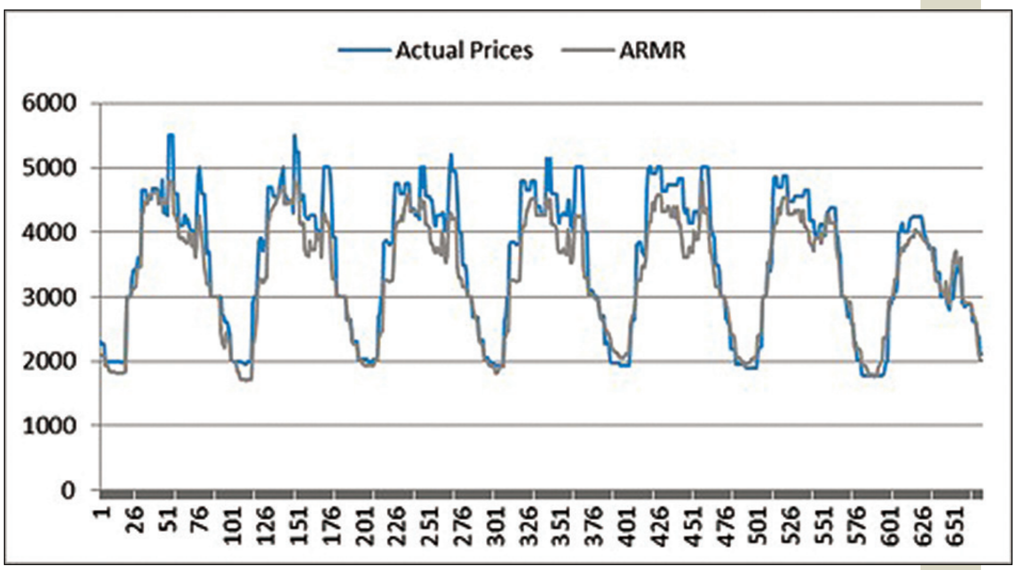


Fig.17. Power Purchase and Sell Bids in Energy Brokerage System

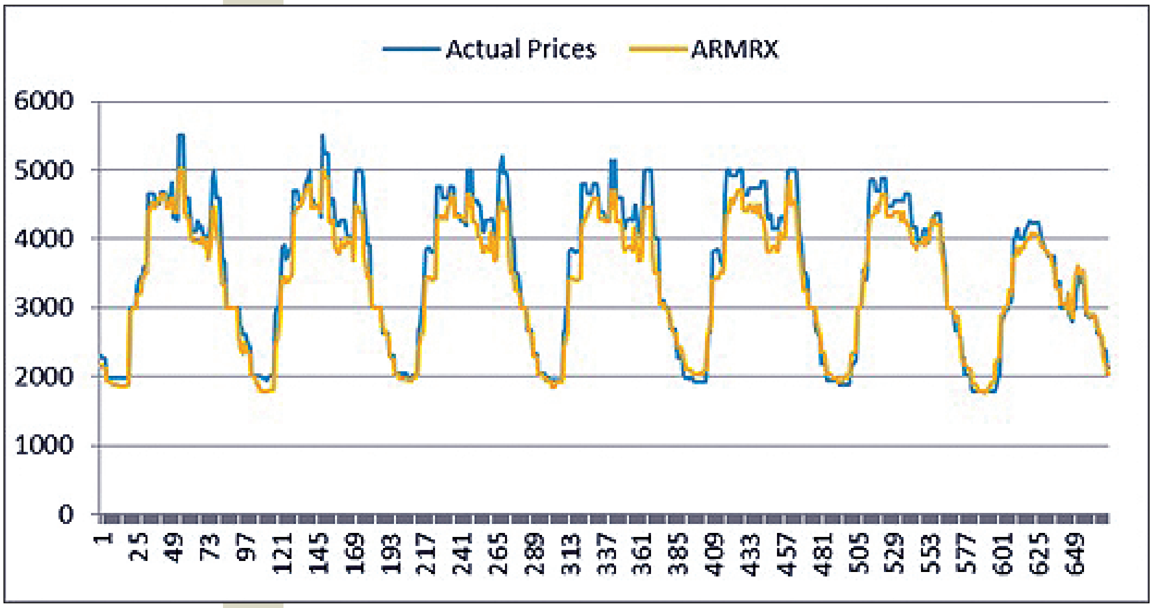


Fig 19. Actual Price vs Forecasted Price of ARMRX Model

Figures 18 and 19 show the actual and forecasted electricity price using ARMR and ARMRX approaches respectively. These are used in the short time power purchases. Table1 shows the error in price forecasting using different methods

TABLE 1. COMPARISON OF ARMR MODEL AND ARMRX MODEL

	ARMR Model	ARMRX Model
MAPE	7.56%	5.40%
Standard Deviation of Errors	7.86%	5.61%
Maximum Error	31.4%	22.5%
Minimum Error	-24.4%	-17.4%

Short Term Power Purchase

In short term power purchase, each utility is interconnected to other utilities and independent power producers who supply electricity to neighboring areas. For an optimal power purchase decision several variables are to be considered.

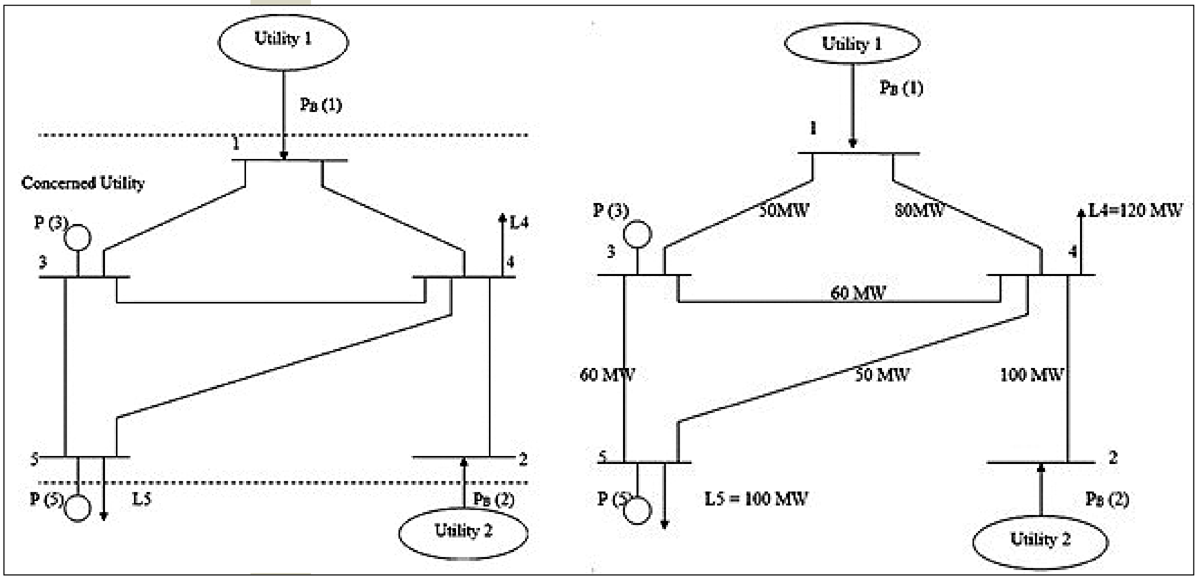


Fig 16. Dynamic Energy Trading using short term power purchase

The load forecasting accuracy that could affect the price decisions in a dynamic electricity environment, the estimate of the market price that could affect the optimal short term generation scheduling in each utility and the network reliability and component availability that could affect the buy/sell decisions as well as the transmission access issues are to be considered. This article describes a new approach to make an optimum buy decision to maximize the utility's operation or minimize the total cost (generation cost and buying cost) considering the uncertainty in prices. The various variables that are considered are the load, the offered prices for power, the line flows and the local generation.

Conclusions and future Work

Dynamic Power Pricing in energy markets is an increasingly important area of research in the current context of real time energy trading in electricity markets. Many parameters influence the performance of the Dynamic Electricity Markets. Load and Price forecasting are important constituents of the study. This research addresses the issues of real time energy trading with price forecasting, market clearing price and decision making. Market price forecasting has become an important daily activity for the deregulation electric power industry. Forecasting the Market Clearing Prices (MCP) of the daily energy market is developed. Based on careful analysis, the model is designed to use only publicly available input data. The forecasting results show that the model is efficient for days with normal trend but for days with price spikes we need to consider a better model.

In future work, dynamic pricing of electricity using peer to peer energy trading using blockchain is a scope for further research.

Dynamic Power Pricing in energy markets is an increasingly important area of research in the current context of real time energy trading in electricity markets. Many parameters influence the performance of the Dynamic Electricity Markets. Load and Price forecasting are important constituents of the study

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Computing for clean energy

ROLE OF COMPUTING IN DEVELOPING CLEAN ENERGY TECHNOLOGIES

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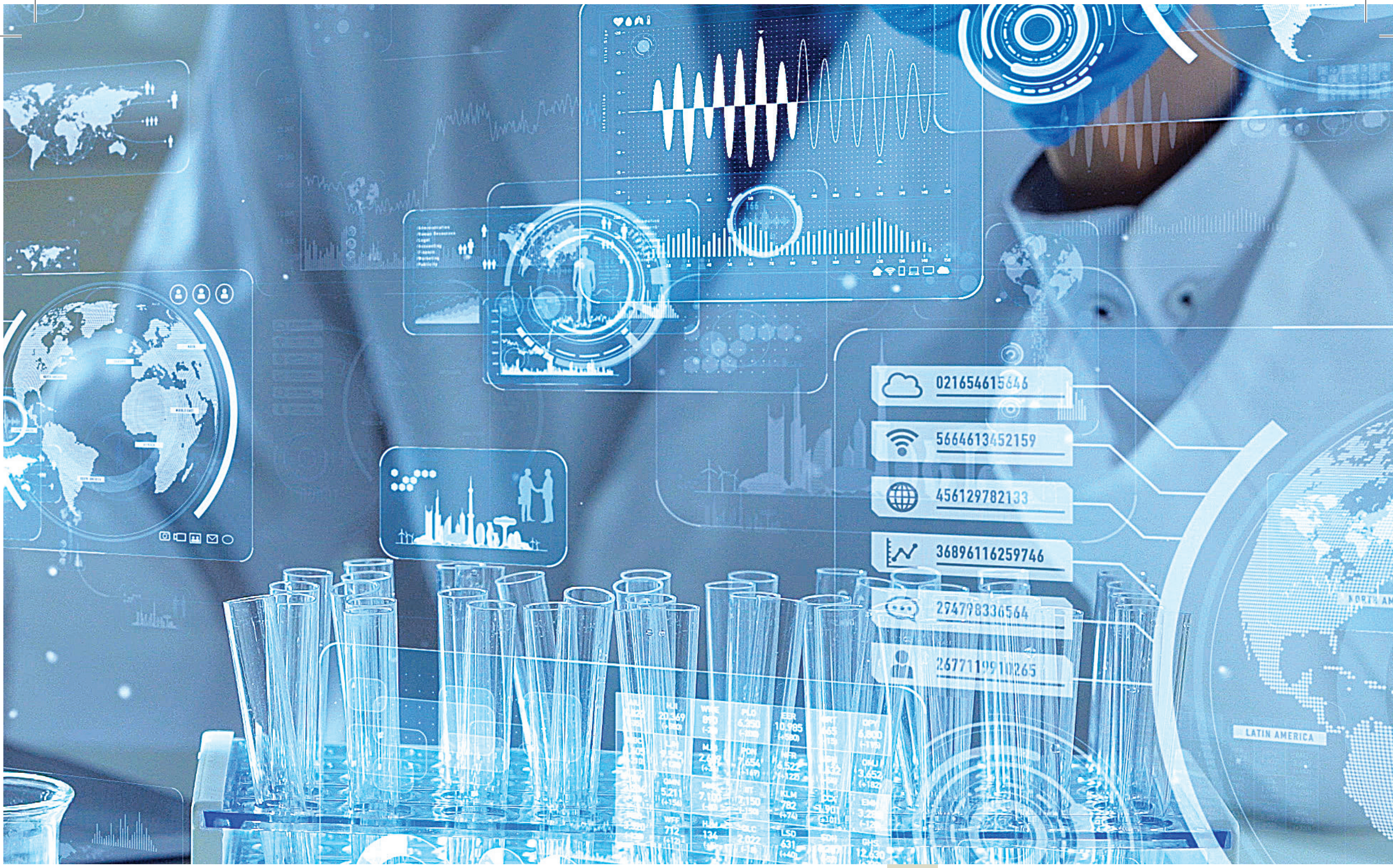

For the past century, chemical engineering has played a crucial role in shaping our lives. Developing a chemical process at the lab scale and taking it to the industrial scale is at the heart of chemical engineering. Of the numerous such processes, converting crude oil into various chemicals and fuels that are the backbone of modern life has been the most instrumental contribution of chemical engineering. However, these chemical processes are also responsible for climate change due to excessive greenhouse gas emissions. There is an imminent need to develop clean processes to produce chemicals and fuels sustainably and environment-friendly. Examples include conversion of biomass to bio-fuels and chemicals, carbon capture utilization and sequestration (CCUS), and electrification. Innovations in novel sustainable and environment-friendly chemical processes require marrying interdisciplinary expertise that did not exist in the recent past.

Historically, developing a new chemical process has involved extensive experimentation at various scales, ranging from a catalyst particle to pilot-scale operations, that require significant time and financial investment. There can potentially be millions of possibilities for a new process at the design stage. Given this vast design space, a trial-and-error approach to experimentation is not practical for identifying the optimal design that is both scalable and economical. Moreover, traditional empirical correlations and design tools are often limited to a narrow range of conditions, making them unsuitable for exploring such a broad design space. Consequently, only a limited number of design parameters are typically examined in conventional approaches, and this limited exploration decides the fate of a new process.

There is a strong need to adopt the rational design approach based on scientific principles in chemical engineering. The transition from empirical toward rational design strategies, however, requires a level of reliability and robustness in the computational

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models that is currently lacking. A major reason for this scenario is the complexity of the problem. Selecting appropriate mathematical models to describe the processes occurring inside a chemical reactor is challenging. Typically, these models are in the form of partial differential equations, which require numerical solution using a computer. Solving these equations for real systems become impractical beyond laboratory scale. At the pilot and industrial scales, analyses often rely on simplistic engineering models that neglect the underlying physics. Examples include equilibrium relations and combinations of ideal reactors, such as continuously stirred tank reactors (CSTR) and plug flow reactors (PFR).

In this context, the recent revolution in high performance computing (HPC) and ML/AI tools can be a gamechanger.

- Supercomputers/High-performance computing (HPC): the speed of the top supercomputer has been doubling every fourteen months for the last two decades
- ML/AI tools: a variety of algorithms are freely available in the form of user-friendly and scalable APIs

Supercomputers can be used to solve detailed mathematical equations (partial differential equations) for larger reactors, providing unprecedented insights into what occurs inside these reactors. Figure 1 shows a schematic of detailed simulations of fixed bed reactors, where each pellet is resolved (PR-CFD), and fluidized bed reactors, where each particle is tracked (CFD-DEM). These simulations allow investigating the coupling among different underlying phenomena, such as chemical reactions, heat and mass transfer, and fluid flow. Such detailed simulations were not feasible a few decades back. The large amount of high-fidelity data generated by supercomputers can be analysed using ML/AI to generate new knowledge and build high-throughput engineering models. These high-throughput models can explore a vast design space quickly, typically within hours. This exploration could lead to innovative reactor technologies and intensified chemical processes, i.e., significantly high energy efficiency, selectivity, productivity, and lower environmental impact. Moreover, these rapid models can be employed to assess the scalability of promising lab-scale reactors. However, these ideas are still in the exploration stage.

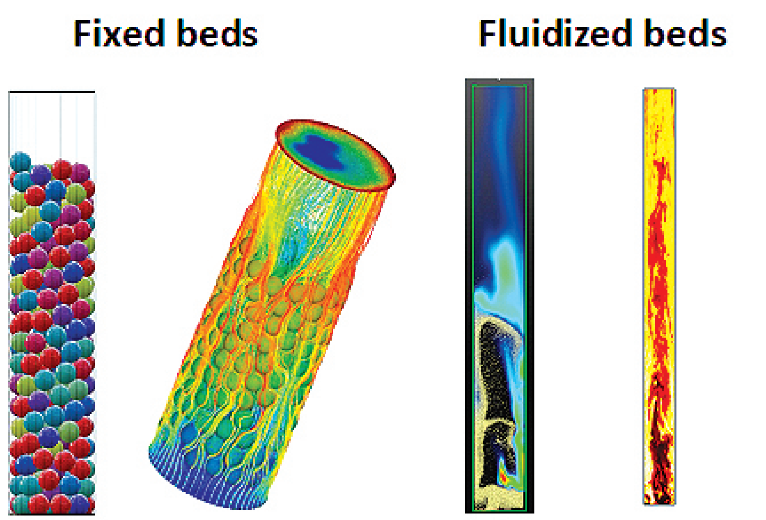

Figure 1: A schematic showing detailed computer simulations of commonly used reactors (fixed and fluidized bed reactors) in the chemical industry. High performance computing (HPC)/supercomputers make it possible to explore multiple physical and chemical phenomena (fluid flow, heat and mass transfer, chemical reactions) from individual particles/pellets to the complete reactor.

India is witnessing a drastic growth in its supercomputing infrastructure, with several supercomputers installed in various parts of the country. These computing facilities can be rented and used to perform simulations. Moreover, several vendors are available that can provide a wide range of CPU and GPU based resources for specific needs of a researcher. Hardware is available; however, we lack on the "soft" side. The penetration of supercomputing and ML/AI advances in core chemical engineering is minimal. Addressing this gap is essential to take advantage of the rapid growth in supercomputing and ML/AI tools.

Most chemical engineering undergraduate and graduate students are not trained in high performance computing and ML/AI tools. Although numerous programs and online materials are available for ML/AI, they are not customized for core engineering disciplines. There is a huge gap between learning ML/AI tools and applying them for core engineering problems, such as building a clean chemical process. Currently there are no dedicated academic curricula let alone training programs that can challenge emerging talent in the country to tackle some of its pressing challenges in energy domain. To this end, focusing on training programs and special conferences targeting this problem is imperative. Academic researchers and industry practitioners who are exploring HPC and ML/AI need to gear up in developing formal training material to train the human resources in this area.

Another challenge is that most experts working on modelling tend to focus on a specific aspect of the problem in silos. For example, they may concentrate on atomic-scale, reactor-scale, or plant-scale process simulations, lacking coordination among these areas. This lack of collaboration hinders the flow of knowledge from bottom (small-scale processes) to top (large-scale processes) and overall goals from top to bottom. For instance, it remains unclear how to connect the discoveries at the catalyst or material level to plant-scale process simulations. Similarly, translating overall objectives from plant-scale process simulations to catalyst/material discovery and improvements is challenging. It is essential to foster collaboration across these domains. Special conferences and courses should be developed to encourage cooperation and knowledge sharing.

Special efforts are needed to build experimental setups to validate computer models. These experiments should be carefully designed so that computer simulations can be rigorously tested. Such experimental setups will bring confidence in the computer models. Currently, many experimental studies either don't provide all the necessary information to simulate them or do not include detailed measurements. Continuous validation against new experiments will improve the applicability of computer models.

Over the years, funding calls have increasingly emphasized the need for measurable outcomes and collaboration with industry. This trend is welcoming, as it suggests that funded projects will foster more academia-industry partnerships. However, the industry-academia-government cooperation need not be limited to advancing technology readiness levels (TRL). There is significant appetite in the industry to engage in collaborative work that involves the development of novel technical approaches and techniques, analytical and computational tools, and methodologies. Often, the scientific and research community can bring about significant advances via physics-based models and scientific computing-based correlations that have higher fidelity and, therefore, much better verifiability and validity.

My lab (Goyal Research

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Group) at IIT Madras is addressing some of the challenges mentioned above. Even though computational modelling has become ubiquitous, its usage is unreliable due to the strong assumptions made in the physical and chemical models. To this end, a multiscale modelling approach is imperative, implying that models at each scale should be developed and rigorously validated against experiments. These validated sub-models are then integrated into the reactor simulations. This multiscale approach contrasts with the current practice of building a model at the largest scale, such as a reactor, with numerous tuning parameters. This approach provides a model that functions well only for a specific experimental setup and within a narrow range of operating conditions (more details are given in Example 1). The multiscale approach makes the modelling "clean," minimizing the need for parameter tuning. Moreover, it can help identify which scale modelling efforts are required. Although multiscale simulations are suitable for a fundamental investigation of a given reactor, they are not optimal for design exploration due to their high computational demand regarding simulation time and HPC requirements.

To this end, ML/AI tools are beneficial. They can help develop data-assisted models that are fast to run and enable rapid exploration of large amounts of data (more details are given in Example 2). Apart from ML/AI, several classical mathematical techniques are available that can reduce the cost of first-principle models. One such technique is numerical homogenization, which allows a complex structure to be represented as an effective medium. In this approach, the physical and chemical models remain the same; only the geometry becomes simpler. For example, a multiphase system can be represented by a porous medium. This simplification makes the meshing straightforward, and only a fraction of mesh elements are required compared to the original model (more details are given in Example 3).

Example 1: Multiscale approach for biomass pyrolysis:

Multiphase reactors, such as fluidized beds, are suitable for large-scale catalytic or non-catalytic thermochemical conversion - pyrolysis or gasification, of biomass and plastic. These reactors exhibit a large separation of scales, ranging from a single particle to the reactor, making their computational and experimental investigation challenging. The small-scale processes, such as chemical reactions and intra-particle phenomena inside a single particle, are strongly coupled with the multiphase reactor hydrodynamics and can have a substantial impact on the reactor performance. To address these challenges, we develop a multiscale computational framework coupling experimentally validated biomass devolatilization kinetics and spatially resolved biomass particle devolatilization model in a CFD–DEM framework. The devolatilization chemistry is represented by the detailed multistep kinetic scheme consisting of 19 solid species, 20 gaseous species, and 24 reactions developed by the CRECK group. Biomass pyrolysis in a fluidized bed reactor at 500 °C is simulated using the developed multiscale model. The impact of particle-scale biomass devolatilization models on the reactor performance was evaluated.

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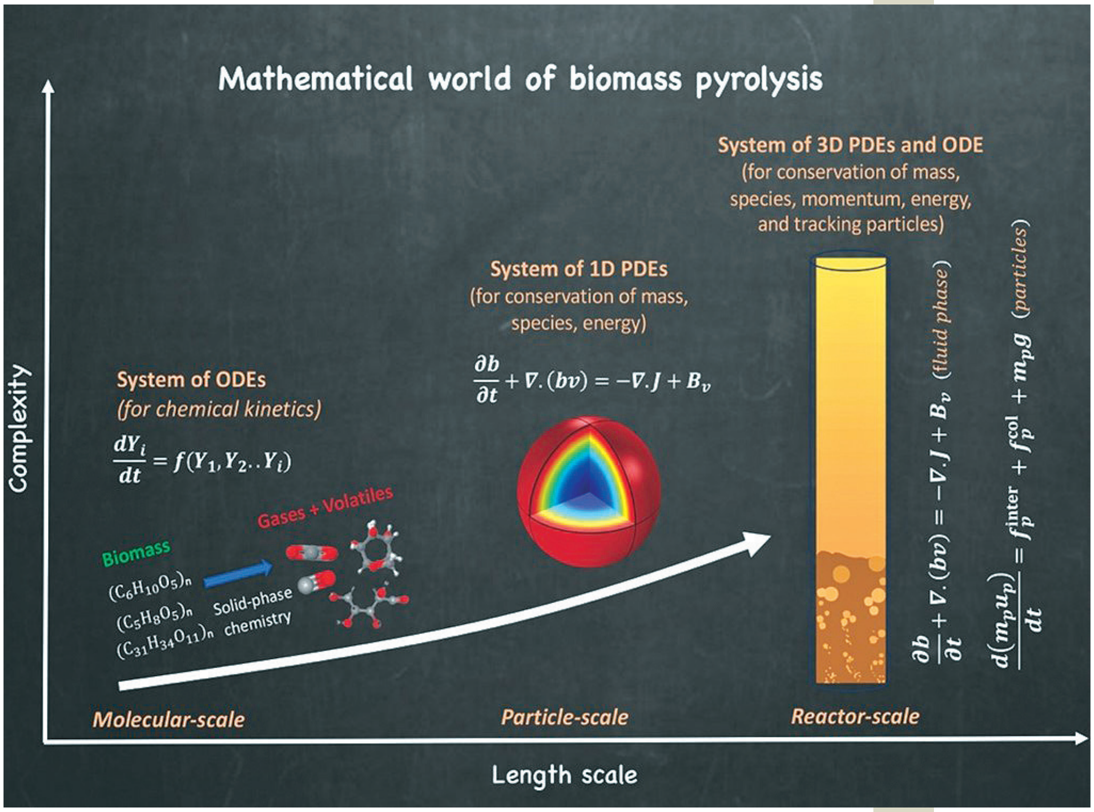

Figure 2: An example of multiscale approach for modeling biomass pyrolysis. Kinetic model for biomass devolatilization chemistry, a one-dimensional intraparticle model for individual biomass particles, and CFD-DEM model for a fluidized bed reactors are validated against experiments and coupled together. [Taken from Kumar and Goyal, React. Chem. Eng., 2024, 9, 2552]

Example 2: ML/AI for data-assisted modelling and data exploration

CFD simulations of chemical reactors using detailed chemical kinetic models are challenging in terms of numerical complexity and run time. Detailed kinetic models include radical species that span a wide range of time scales, making the resulting system of ODEs stiff. Solving a large, stiff system of ODEs in multiphase CFD simulations puts a strict restriction on the time step, rendering such simulations impractical even for laboratory-scale reactors. Moreover, these simulations face convergence issues. For this reason, most reactor CFD simulations rely on global kinetics, even when detailed kinetic schemes are available. To address these challenges, we developed a gated recurrent unit (GRU) based recurrent neural network (RNN) model to predict the reactants and product evolution along a fluidized bed reactor length. The developed ML model is applied to predict biomass thermochemical conversion at 800–1000 oC in a fluidized bed reactor. Biomass devolatilization and gas-phase chemistries are represented by kinetic schemes comprising 20 species with 24 reactions and 39 species with 118 reactions, respectively. Generating a large amount of training data needed to train the GRU-RNN model directly from CFD simulations is impractical. To this end, reactor network models comprising ideal reactors are used to generate the training data. A wide range of biomass compositions and operating conditions are used, ensuring model generality. The developed ML model predictions are in reasonable agreement with the expensive CFD-DEM simulations. The ML model reduces the computational cost of CFD-DEM simulations by 10 orders of magnitude. Figure 3 provides a schematic of the overall methodology.

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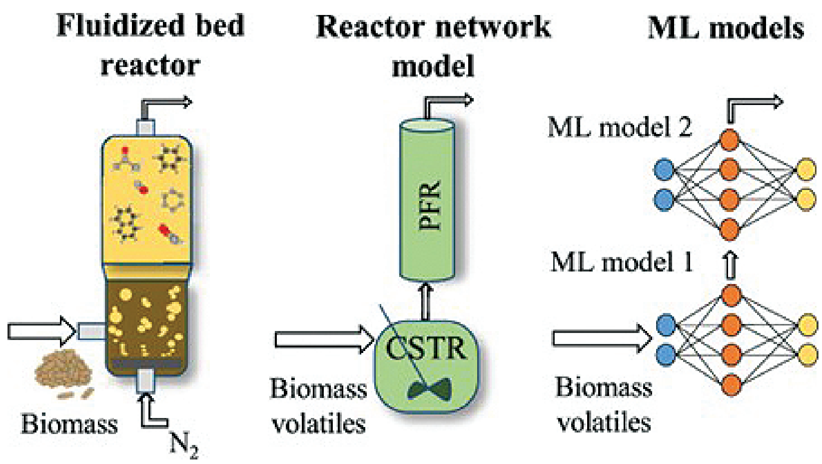

Figure 3: Schematic showing how ML can be used to build fast models for complex chemical reactors. [Taken from Kumar et al., Ind. Eng. Chem. Res. 2025, 64, 2, 999–1010.]

In addition to developing fast data-assisted models, ML can be used to explore and analyze the large amount of data generated from computer simulations. We recently deployed DBSCAN – an unsupervised machine learning technique, to capture multiphase features, such as bubbles in a fluidized bed reactor

In addition to developing fast data-assisted models, ML can be used to explore and analyze the large amount of data generated from computer simulations. We recently deployed DBSCAN – an unsupervised machine learning technique, to capture multiphase features, such as bubbles in a fluidized bed reactor. The methodology is user-friendly and scalable. Figure 4 shows representative results, where Fig 4a shows the visualization made in commercial software (ANSYS Ensight), and Fig 4b shows the prediction of DBSCAN-based methodology. Apart from visualization, the technique provides all the statistics related to the bubbles, such as size, shape, surface area, volume, and maximum chord length. We are working on extending this technique to other complex multiphase reactors.

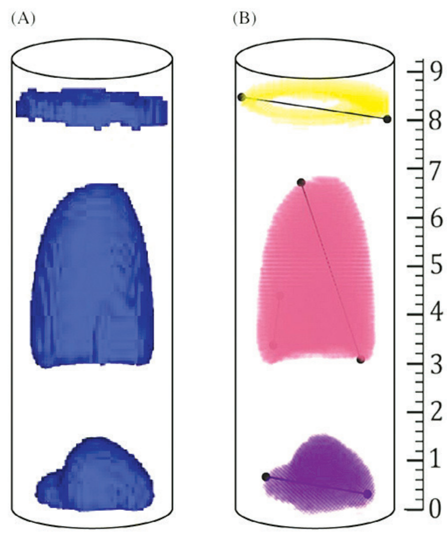

Figure 4: Schematic demonstrating the utility of unsupervised machine learning algorithms in identifying bubbles and obtaining their properties from CFD simulations of a fluidized bed reactor. [Taken from Kumar and Goyal, AIChE J. 2024, 70:e18360.]

Example 3: Fast reactor models using homogenization:

The large separation of length scales in multiphase chemical reactors from an active catalyst site to the entire reactor makes simulations computationally expensive. This issue can be addressed with homogenization methodology by developing physics-based high throughput models. This technique transforms the point-wise mathematical description into averaged equations utilizing the effective medium properties. The computational cost associated with the homogenized (effective) phase is much lower than that of the original multiphase system.

We have successfully employed this approach for monolith reactors and microwave heating. Figure 5 illustrates the central concept behind this technique. Detailed simulations of a unit cell are performed, and the resulting simulation data is used to evaluate effective medium properties, such as permittivity and thermal conductivity, needed for the averaged equations. By employing this method, we achieve several orders of magnitude reduction in the number of mesh elements and simulation time. At the same time, the overall three-dimensional profiles can still be obtained as predicted by the detailed simulations. We are extending this methodology to more complex reactors, such as fixed beds, where particle-resolved simulations are extremely challenging to perform.

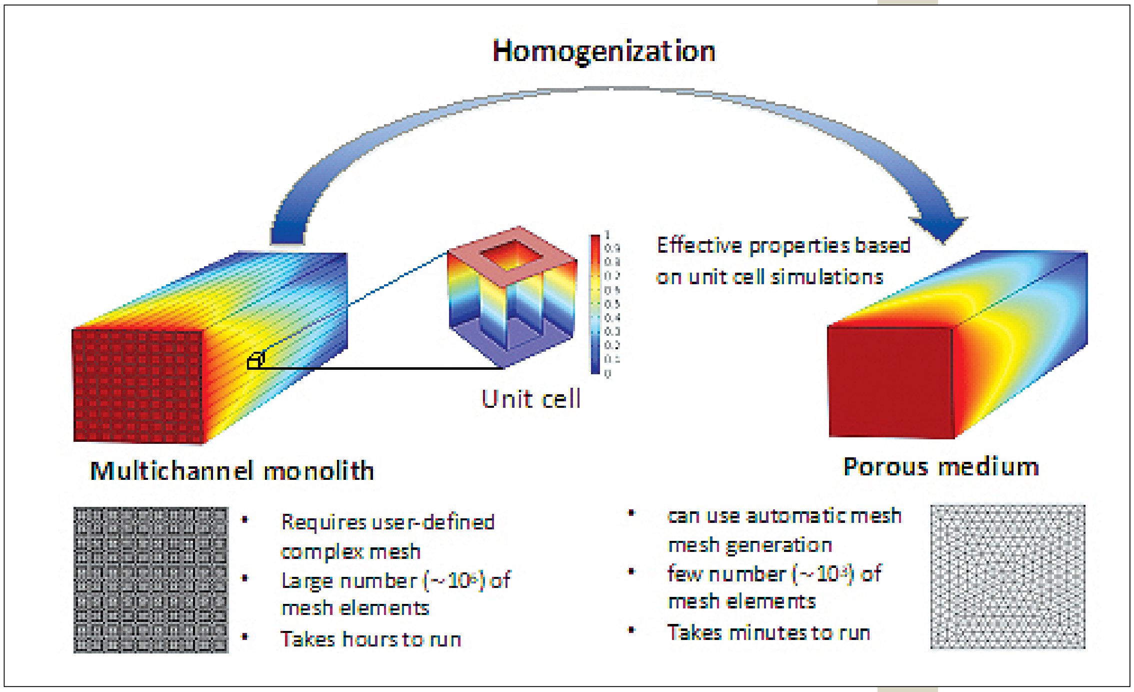

Figure 5: Schematic of how homogenization can be used to represent a complex multiphase system as a simple porous medium. This approach can be used for structured reactors and fixed bed reactors, making their optimization feasible. [Adapted from Kavale et al., Ind. Eng. Chem. Res. 2023, 62, 45, 19004-19018]

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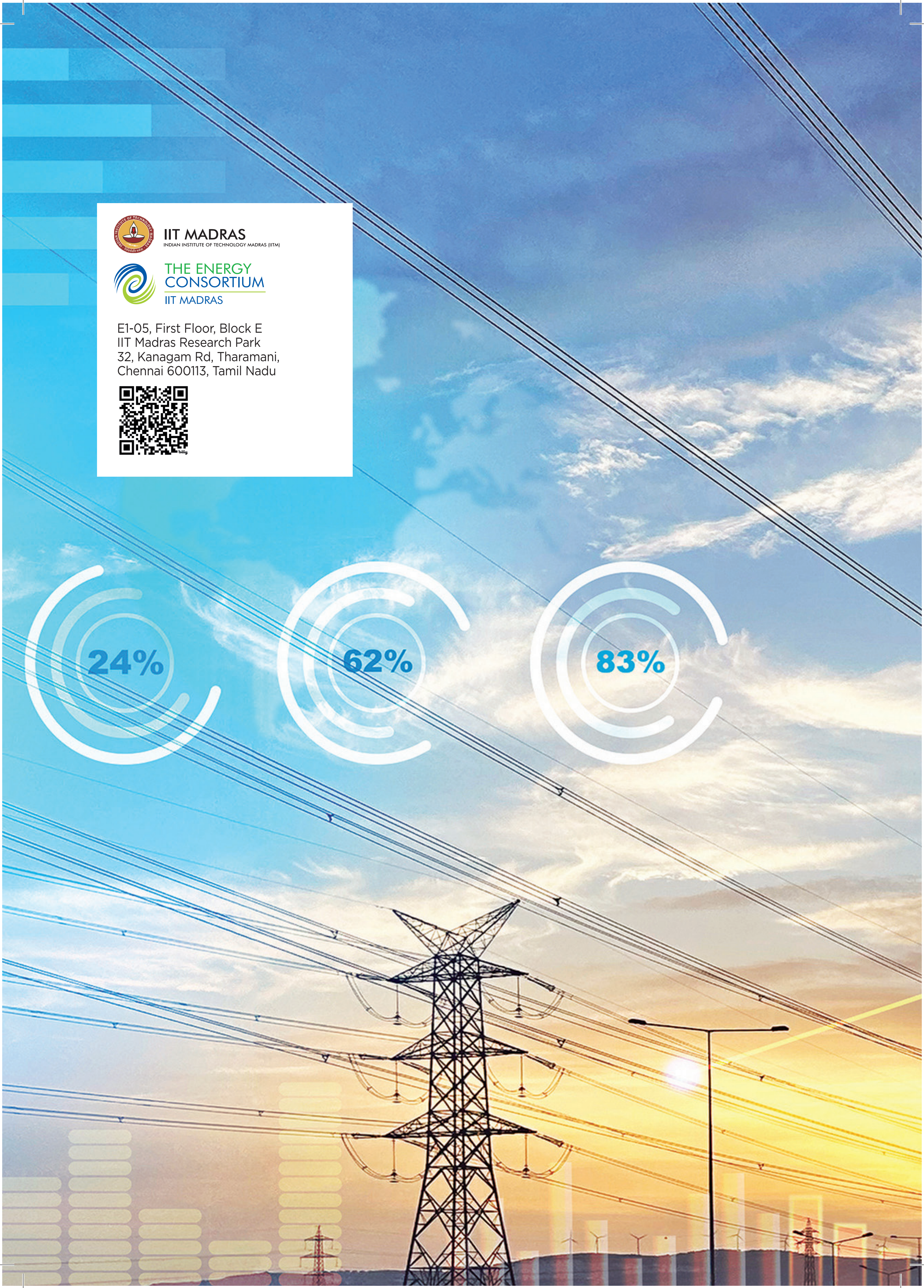

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