Artificial Intelligence in Process Systems Engineering: Quo Vadis?

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AI for Industry 4.0 in PSE

- Industry 4.0
- Digital 4.0
- Digitalization of Manufacturing
- Internet-of-Things (IoT)
- Smart and autonomous systems fueled by Data and AI

- All sounds very new, right?

Source: Wiki
AI for Industry 4.0 in PSE

• But AI in PSE is not new!
  • Has a 35-year-old literature: >3000 papers

• Review AI in PSE: 1980s to Present

• Potential of AI in PSE: Present – 2040?

• Identify the challenges and opportunities
  • Conceptual, Implementational, Organizational

• Broad overview
  • Not a detailed technical presentation
  • More details in my paper

The Promise of Artificial Intelligence in Process Systems Engineering: Is it here, finally?
V. Venkatasubramanian, AIChE Perspective Paper, Feb 2019
What is AI?

“Artificial Intelligence is the study of how to make computers do things at which, at the moment, people are better.”

Branches of AI

• Games - study of state space search, e.g., Chess, Go
• Symbolic math - e.g., MACSYMA, Mathematica
• Robotics – e.g., Self-driving cars
• Vision – e.g., Facial recognition
• Natural language processing (NLP) and semantic modeling, e.g. Siri
• Hardware for AI – e.g., Symbolics LISP Machines, GPUs
• Distributed & Self-organizing AI – e.g., Drone swarms, Agents
• Expert Systems or Knowledge-based Systems
• Machine Learning (ML) – e.g., Bayesian classifiers, Deep neural nets
Promise of AI in PSE

• AI is essentially about problem-solving and decision-making under complex conditions
  • Ill-posed problems
  • Model and data uncertainties
  • Combinatorial search spaces
  • Nonlinearity and multiple local optima
  • Fast decisions are required – e.g., fight or flight responses

• But these are applicable to many PSE problems: Design, Synthesis, Control, Optimization, Safety

• So some of us went about developing AI approaches in the early 1980s
• We expected significant impact from AI, much like from Optimization and Model Predictive Control (MPC)
• But it did not happen – Why?
AI in PSE:
Why very little impact so far?

Before I answer this question, let me first review the different phases of AI in PSE.
AI in PSE: Phase I


Key ideas
• Separation of domain knowledge from inference
• Flexible execution order of program
• IF-THEN Rules for Procedural Knowledge
• Semantic networks for Taxonomies

MYCIN: Expert system for diagnosing infectious diseases (1972-82)
• Stanford Computer Science and Medical School Project
• Knowledge base: ~600 rules
• Diagnosed better than the physicians

Image source: https://www.tutorialspoint.com/artificial_intelligence/artificial_intelligence_expert_systems.htm
AI in PSE: Phase I

- DECADE (1985) Westerberg: Catalyst Design
- MODEX (1986) Venkatasubramanian: Fault Diagnosis
- DSPL (1988) Davis: Distillation Column Design

- First course on AI in ChE, taught at Columbia (1986)
- First conference on AI in ChE, held at Columbia (1987)

Expert Systems Drawbacks
- Too much time, effort, and specialized expertise
- Did not scale well for industrial applications
AI in PSE: Phase II

• Machine Learning I - Neural Networks (~1990 – ~2005)

Key idea
• Backpropagation algorithm (1986)
• Bottom-up strategy
• Automatically learned patterns between input and output vectors by adapting the weights

Nonlinear Function Approximation and Classification Problems

Most applications in ChE were in process control and fault diagnosis with some industrial applications

Collaborative Decision Support for Industrial Process Control

A Proposal to NIST Advanced Technology Program

Ohio State
(Davis)

Purdue
(Venkatasubramanian)

University of Toronto
(Kim Vicente)

USD $17,000,000
(49% matched back)

Fore-runner to the Smart Manufacturing Initiative (2016)
• Implemented in G2, tested at Exxon (Baton Rouge)
• **Dkit** successfully anticipated and diagnosed several failures even before the alarms went off (~1/2 – 2 hours ahead)
• **Dkit** was licensed to Honeywell in 1998
• Little impact beyond the prototype: Implementational and Organizational difficulties
• **We were about 20-30 years too early** for practical impact!

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Mylaraswamy, Dinkar, **DKit: A Blackboard-based, Distributed, Multi-Expert Environment for Abnormal Situation Management**, Purdue University, PhD Thesis, **1996**.

**Forward Problem**
- Prediction of Performance
- First Principles + Neural Nets

**Inverse Problem**
- Prediction of Structure or Composition
- Genetic Algorithm (Directed Evolution)


- **Frances Arnold (Caltech)**
- Directed Evolution *in vitro*
- Awarded the Nobel Prize in Chemistry in 2018

- **Fuel Additives** (Lubrizol, 1995-99)
- **Rubber Compounds** (Caterpillar, 1998-2000)
Reaction Modeling Suite: 
AI-based Modeling Environment for 
Catalyst Development (2002-05)

Novel features
• Domain-specific language for reaction chemistry
• Domain-specific compiler
• Chemistry Ontology
• Active Learning

## Chemistry Rules for Propane Aromatization on HZSM-5

<table>
<thead>
<tr>
<th>Chemistry Rules</th>
<th>Representative Chemical Reactions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Alkane adsorption</td>
<td><img src="image1" alt="alkane adsorption" /></td>
</tr>
<tr>
<td>2. Alkane desorption</td>
<td><img src="image2" alt="alkane desorption" /></td>
</tr>
<tr>
<td>3. Carbonium ion protolysis</td>
<td><img src="image3" alt="carbonium ion protolysis" /></td>
</tr>
<tr>
<td>4. Carbonium ion dehydrogenation</td>
<td><img src="image4" alt="carbonium ion dehydrogenation" /></td>
</tr>
<tr>
<td>5. Olefin adsorption</td>
<td><img src="image5" alt="olefin adsorption" /></td>
</tr>
<tr>
<td>6. Olefin desorption</td>
<td><img src="image6" alt="olefin desorption" /></td>
</tr>
<tr>
<td>7. Aromatization</td>
<td><img src="image7" alt="aromatization" /></td>
</tr>
<tr>
<td>8. Beta-Scission</td>
<td><img src="image8" alt="beta-scission" /></td>
</tr>
<tr>
<td>9. Hydride Transfer</td>
<td><img src="image9" alt="hydride transfer" /></td>
</tr>
<tr>
<td>10. Oligomerization</td>
<td><img src="image10" alt="oligomerization" /></td>
</tr>
</tbody>
</table>
**Reaction Modeling Suite (RMS): Domain-specific Ontology, Language, and Compiler**

**English Language Rules**

**Chemistry**
8. Beta Scission
   transforms a carbenium ion into a smaller carbenium ion and an olefin

**Grouping**

8. a. Formation of a secondary carbenium ion
   is 20 times faster than a primary carbenium ion
8. b. Formation of a tertiary carbenium ion
   is 60 times faster than a primary carbenium ion

**Reaction Description Language Plus**

**Beta Scission**
- Label-site c1+ (find positive carbon)
- Label-site c2 (find neutral-carbon attached-to c1+)
- Label-site c3 (find neutral-carbon attached-to c2)
- Forbid (primary c3)
- Forbid (less-than (size-of reactant) 9)
- Disconnect c2 c3
- Increase-order-of (find bond connecting c1+ c2)
- Add-charge c3
- Subtract-charge c1+

**Model Generator**

**Beta Scission**
- Label-site c1+ (find positive carbon)
- Require (c1+ primary and product)
  set-k k1
- Label-site c2+ (find positive carbon)
  Require (c2+ secondary and product)
  set-k 20*k1
- Label-site c3+ (find positive carbon)
  Require (c2+ tertiary and product)
  set-k 60*k1

**Mathematical Equations**
\[
\frac{dC_A}{dt} = -k_1 C_A \\
\frac{dC_B}{dt} = k_1 C_A + k_2 B - k_5 C_B \\
\theta_A + \theta_B + \theta_C = 1
\]

100’s of DAE’s

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Catalyst Design (2002-05): Guided Experimental Design and Model Development

Re-discovered recently as Active Learning

Formulation of Experiments

High Throughput Experiments

Human Expert

Chemistry Rules

Reaction Modeling Suite

Performance Curves

Rate/Selectivity vs. time

Feature Extraction

Model Refinement

AI Applications in PSE  
(1983 – 2010)

- Process monitoring and fault diagnosis
- Process control
- Process design
- Process synthesis
- Process safety analysis
- Optimization
- Planning
- Scheduling
- Materials design

- Prototypes demonstrated in all these areas
- Even some industrial applications fielded
So, why was AI not impactful in PSE during (1983-2010)?

- Researchers made great progress on conceptual issues
  - Showed how to formulate and solve these challenging problems
- But we were greatly limited by implementation and organizational difficulties for practical impact
  - Lack of computational power and computational storage
  - Lack of communication infrastructure – No Internet, Wireless
  - Lack of convenient software environment
  - Lack of specialized hardware – e.g., NVIDIA GPU for simulations
  - Lack of data
  - Lack of acceptance of computer generated advice
  - Costs were prohibitive
- Essentially, it took too much effort, time, and money to field industrial applications
- We were too early, by about 20-30 years!
What is Different Now?

- **Cray-2 Supercomputer (1985)**
  - 1.9 GFLOPS
  - 244 MHz
  - 150 KW!
  - $32 Million! (2010 dollars)

- **Apple Watch (2015)**
  - 3 GFLOPS
  - 1 GHz
  - 1 W!
  - $300!

- Performance/unit cost Gain ~150,000x

Source: Wiki
How Did this Happen?

- Basically Moore’s Law happened over the last ~50 years!

- All these metrics improved by orders of magnitude!
  - Computational power
  - Computational storage
  - Communication infrastructure: Internet, Wireless
  - Convenient software infrastructure – Python, Java, OWL, ...
  - Specialized hardware – graphics processors (GPUs)
  - Big Data
  - Trust & Acceptance – Google, Yelp, Trip Advisor, Tinder, ...

- It has become much easier and cheaper to develop AI-based solutions

Source: Wiki
AI in PSE: Entered Phase III (2005-?)

- Phase III: Machine Learning II - Data Science (2005 – Present)
  - Convolution or Deep Nets
  - Reinforcement Learning
  - Statistical Machine Learning
- Key idea: Hierarchical feature extraction and feature combination
- Important techniques, but not really new!
- What is really new are Data, GPU, and Software
- Big impact in NLP, Robotics, Vision
  - Watson, Siri, Alexa, AlphaGo, Self-driving cars
Data Science and Machine Learning:  
Hype vs Reality  

• First of all, there is a lot of reinventing the wheel going on  
• Many of the “new” techniques are really old ideas from 20-30 years back  
  • “Look, Ma, No Hands” self-driving car project at CMU  
  • Minivan steered itself for 2,800 of the 2,850 miles between Pittsburgh and San Diego in July 1995  
  • Convolutional neural networks are from 1990  
  • Autoencoder neural networks are from 1991  
  • Inverse design of materials using directed evolution is from 1992  
  • Causal models and Explicable AI date from the early 1990s  
  • Hybrid models combining first-principles with data-driven techniques are from 1995  
• It’s worth reading the old papers!
Data Science and Machine Learning Now: Hype vs Reality

• Second, one doesn’t necessarily need convolutional networks, reinforcement learning, etc., for many problems in ChE
  • Other simpler and more transparent AI techniques are often adequate

• Third, how do we leverage the great amount of prior knowledge that we already have about our materials, processes, and systems?
  • ChE is different from game playing, vision, and speech
Importance of Causal Mechanisms and Hybrid Models

- Osco Drugs Diaper-Beer Correlation
  - People who bought diapers also bought beer
  - Osco didn’t care why, but was happy to profit from it
- However, in many ChE applications we would like to know why something works from a mechanistic perspective
- No fundamental laws behind the Diaper–Beer relationship
- But in science and engineering there most certainly are
- Mechanism-based causal explanations are at the foundations of science and engineering
Lack of Mechanistic Understanding

• Self-driving car can navigate impressively through traffic, but does it “know” and “understand” the concepts of mass, momentum, acceleration, force, and Newton’s laws, as we do?
  • It does not
  • Its behavior is like that of a cheetah chasing an antelope in the wild
  • Both animals display great mastery of the dynamics of the chase, but do they “understand” these concepts?

• Current AI systems have perhaps achieved animal-like mastery of their tasks, but they have not gained deeper “understanding” as many humans do

• Mechanistic causal understanding is important in many ChE applications such as diagnosis, control, and safety to build credibility
Going Forward:

Challenges and Opportunities
Challenges and Opportunities in PSE: “Easy” Applications of AI

• Large amounts of Data + Easy to use ML tools
• Routine applications, can be done now
• Process Operations
  • Oil-well performance monitoring
  • Wind turbines monitoring
  • Process intensification
  • Preventive maintenance
• Material Science
  • Estimating physical properties from structures/compositions
  • Determination of structural features
  • Nanoparticle packing
  • Reaction path prediction ..... 
• Lots of recent industrial applications in this category
Challenges and Opportunities in PSE: “Hard” Applications of AI

- **Hybrid AI Models**
  - First-Principles + Data-driven
  - Building Physics and Chemistry into Data-driven models

- **Causal models**
  - Building cause-and-effect relationships for generating explanations and insights

- **Signed Digraph (SDG) Models**
  - Will take ~10 years to do routinely, systematically, and correctly
Challenges and Opportunities in PSE: “Harder” Applications of AI

• “Watson”-like systems
• Domain-specific Ontologies
• Languages
• Compilers ...
• Will take ~10-20 years
How about “Watson” for PSE?

• What will it take to develop “Watson” for PSE?

  • Not just qualitative facts
  • Quantitative
  • Math Models
  • Charts, Tables, Spectra
  • Heuristic Knowledge
"Watson" for Pharmaceutical Engineering (Prototype 2005-2011)

**Modeling**
- Multiscale models for synthesis methods
- Modeling and Analysis: Crystalline Structure
- Unit Operation models: DEM/CFD/FEM
- Process modeling: First Principles Process Model

**Material Science**
- Material synthesis method development
- Systematic functionalization
- Control methodology for spatial structure of organic composites
- Determine structure-function-performance relationships

**Tools for Design and Manufacturing**
- Intelligent Systems for Preformulation Formulation
- Spatial Structure
- Process Monitoring and Control
- Optimization, Simulation, Safety Analysis, Scheduling

**Process**
- Crystallization, Granulation, Drying, Size Reduction etc.
- Equipment: Blender, tabletting press, roller compactor, fluid bed

**Organic composites: Physical Properties**
- Powder Properties

**Knowledge relationships**

**Ontological Informatics Infrastructure**

**Dissolution Problems**

**Instruments**
- "Watson" for Pharmaceutical Engineering (Prototype 2005-2011)

Purdue Ontology for Pharmaceutical Engineering
2006-2011

Decisions

Knowledge

Models

Information

GUI

Computational tools

Unstructured information

**Management of Math Models: OntoMODEL**

Summary
Phases of AI in PSE


• Phase II: Neural Nets (1990-2005)

• Phase III: Data Science (2005 - ?)
Knowledge Modeling in ChE: Evolution of Three Paradigms

- **Differential-Algebraic Equations (DAE):** Amundson Era (1950s)
  - Modeling Process Units
  - Modeling First-principles

- **Optimization (MILP, MINLP):** Sargent Era (1970s)
  - Modeling Process Engineers: Decision-making
  - Modeling Constraints

- **Artificial Intelligence**
  - Westerberg, Stephanopoulos, and others (1980s)
    - Modeling Process Engineers & Data: Decision-making
    - Modeling Symbolic Structures and Relationships
Challenges and Opportunities in PSE: “Easy”, “Hard”, and “Harder”

• Category “Easy”: Routine applications, can be done now
  • Large amounts of Data + Easy to use ML tools
  • Lots of recent industrial applications of this category

• Category “Hard”: ~10 years
  • Hybrid AI Models: First-Principles + Data-driven Models
  • Causal models

• Category “Harder”: ~10-20 years
  • “Watson”-like systems in ChE
  • Domain-specific Ontologies, Languages, Compilers, …
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Questions?