AI-based Modeling Software for Amine and Degradation Product Emissions

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Reaction Engineering International

Privately held consulting firm recognized for independent analysis and evaluations involving a range of industrial combustion applications

- Technical focus on multi-phase, chemically reacting flows
- Serving the industries since 1990
- Affiliates in Asia and Europe
- Established capabilities include advanced modeling, process evaluation and testing

Phase I Technical Objectives

1. ML Model Development and Validation

2. ML Model Demonstration in a Real-time Operation within a Plant's DCS system

3. ML Model Demonstration in a Decision-making Framework based on IDAES

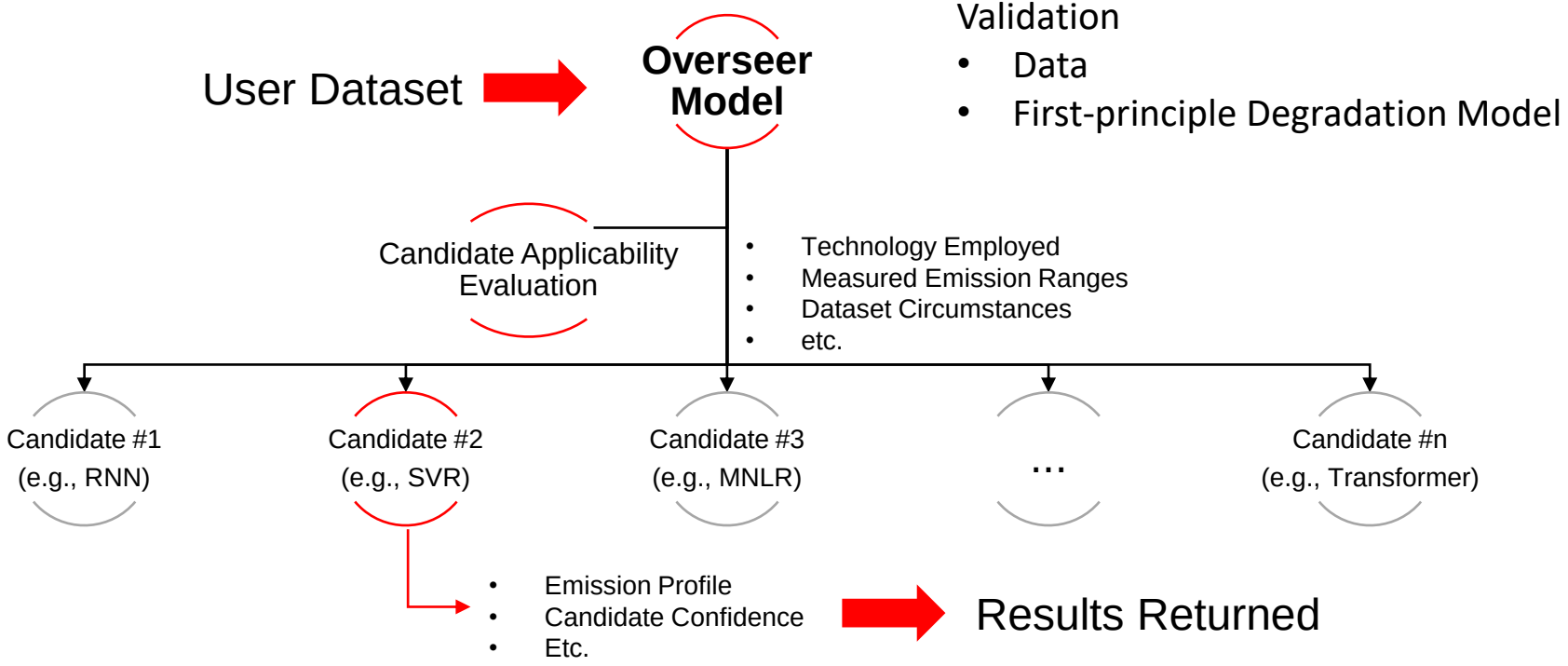
Phase I Work Plan

	Task	Project Month											
		1	2	3	4	5	6	7	8	9	10	11	12
1	Program Management and Reporting												
2	Aquire Training Data			1									
3	Implement Machine Learning Engine and Train Model							2					
4	Implement Prototype first principles model												
5	Validate Model										3		
6	Demonstrate ML model with process control software												
7	Demonstrate ML model in PowerGenExpert®												4

Project milestones include:

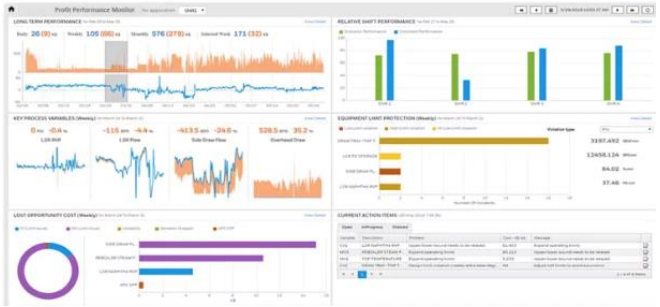
- Milestone 1 – Data acquisition from TCM
- Milestone 2 – Completion of ML model development and training
- Milestone 3 – Completion of model validation
- Milestone 4 – Completion of the integration of the ML model with PowerGenExpert

AI Framework



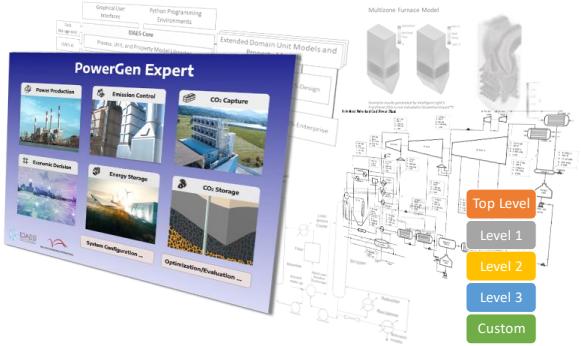
Demonstration in …

- Real-time Process Control
  - Integration with existing process control system
  - Demonstrate the model's ability to control and optimize the process in real time



Example:
https://process.honeywell.com/us/en/initiative/advanced-process-control/advanced-process-control

- PowerGen Expert
  - Next-generation, hybrid energy decision-making software with economic analysis, including carbon capture technology (SBIR Phase II)
  - Implement/Demonstrate the model to predict emissions and guide best operational practices for solvent management



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- DOE/NETL Project Manager: Katharina (Katy) Daniels

Overview of the Phases

Phase I

- Obtain target data to train ML model
- Develop machine learning engine
- Train ML model
- Validate ML model
- Deploy and demonstrate ML model on DCS common to industry
- Integrate and demonstrate ML model with state-of-the-art hybrid energy systems modeling framework

- REI
- Taber (Dr. Jacob Tuttle)

Phase II

- Obtain additional datasets
- Refine machine learning engine
- Train and validate ML models
- Add first principles modeling
- Add optimization capabilities for exploring best solvent management practices
- Implement a DCS-ready version for commercial use
- Pilot-scale demonstration
- Fully implement ML model(s) into REI's hybrid energy systems modeling framework

- REI
- Taber (Dr. Jacob Tuttle)
- Brigham Young University (pilot-scale carbon capture)
- Industrial partners

Phase III

- Model performance optimization
- Integrate with various plant control systems
- Experimental campaign for further validation, ML models
- Commercial-scale demonstration
- Commercialization

- REI
- Taber (Dr. Jacob Tuttle)
- Industrial partners
- Equipment suppliers
- Private investors