From Flowsheet to AI: Building Reproducible Open-Source Process Engineering Workflows with DWSIM and Python

Dr. Nitin Dutt Chaturvedi

Assistant Professor

Department of Chemical and Biochemical Engineering

Indian Institute of Technology Patna, India-801106

My profile

Collaborators

Total Publications (From IIT Patna)		
1	Total journal publications in peer reviewed journals	33 (25)
2	Total impact factor of journal publications	250+ (210+)
3.	Highest impact factor of journal publications	15.9 (15.9)
4	Total Conference publications	23 (20)

Research Interests

Transportation Networks **Heat-Water Integration**
Robust optimization
Energy Scheduling

Process Integration **Pinch Analysis**
Batch operations
Generation Planning

Resource Targeting
Modelling and Simulation of Chemical processes

Research Students Details		
1	**Completed (PhD)** Dr. Rakesh Kumar Sinha Dr. Gaurav Shukla Dr. Shubham Kr. Singh Dr. Alquma Haider	4
2	**Ongoing(PhD)** Mr. Manish Meena Mr. Nirvesh Patel Mr. Animesh Kumar	2
3	**Completed M. Tech (by research)** Mr. Piyush Kumawat Mr. Rahul Sudhanshu	2
4.	**Ongoing(M. Tech)** Mr. Abhishek Raj Shekhar	1

JRF Details	
Asit Das (Ongoing)	1

Projects and funding

1	Projects Funding Received (in Lakhs Rs) Early Career Research Award Core Research Grant DST (CCUS)	 22.36 26.88 81.4
2	Number of projects received	3
3.	Number of projects (in submission)	2

Overview: IIT Patna

IIT Patna's campus is located at Amhara, Bihta, 35 km from Patna

Programs Offered: B.Tech, M.Tech, M.Sc, and Ph.D. programs in engineering, science, and humanities

IIT Patna has ten departments:

- ❑ Computer Science and Engineering
- ❑ Electrical Engineering
- ❑ Mechanical Engineering
- ❑ Civil and Environmental Engineering
- ❑ **Chemical and Biochemical Engineering**
- ❑ Materials Science and Engineering
- ❑ Mathematics
- ❑ Physics
- ❑ Chemistry
- ❑ Humanities and Social Sciences

Chemical and Biochemical Engineering

- **B.Tech, M. Tech and PhD Programs**
- 11 Faculties
- 6 Supporting staffs
- **200+ UG students,15+ PG Students, 30+ PhD Students**

Dr. Anoop K Gupta
Computational Fluid Dynamics, Energy Storage, Phase Change Materials

Dr. Atanu K Metya
Molecular Modeling, Interfacial Phenomena, Computational Drug Design

Dr. Jose V Parambil
Crystallization, Separation Processes, Process Development

Dr. Mahendra Ram
Thermochemical Treatment, Water Treatment, Nutrition Extraction

Dr. Lalita K Shekhawat
Bioprocessing, Bioseparation, Computational Fluid Dynamics

Dr. Nitin D Chaturvedi
Process System Engineering, Modeling and Simulation, Optimization

Dr. Sandip Khan
Wetting and Interfacial Properties, Phase Behavior, Evaporation and Condensation

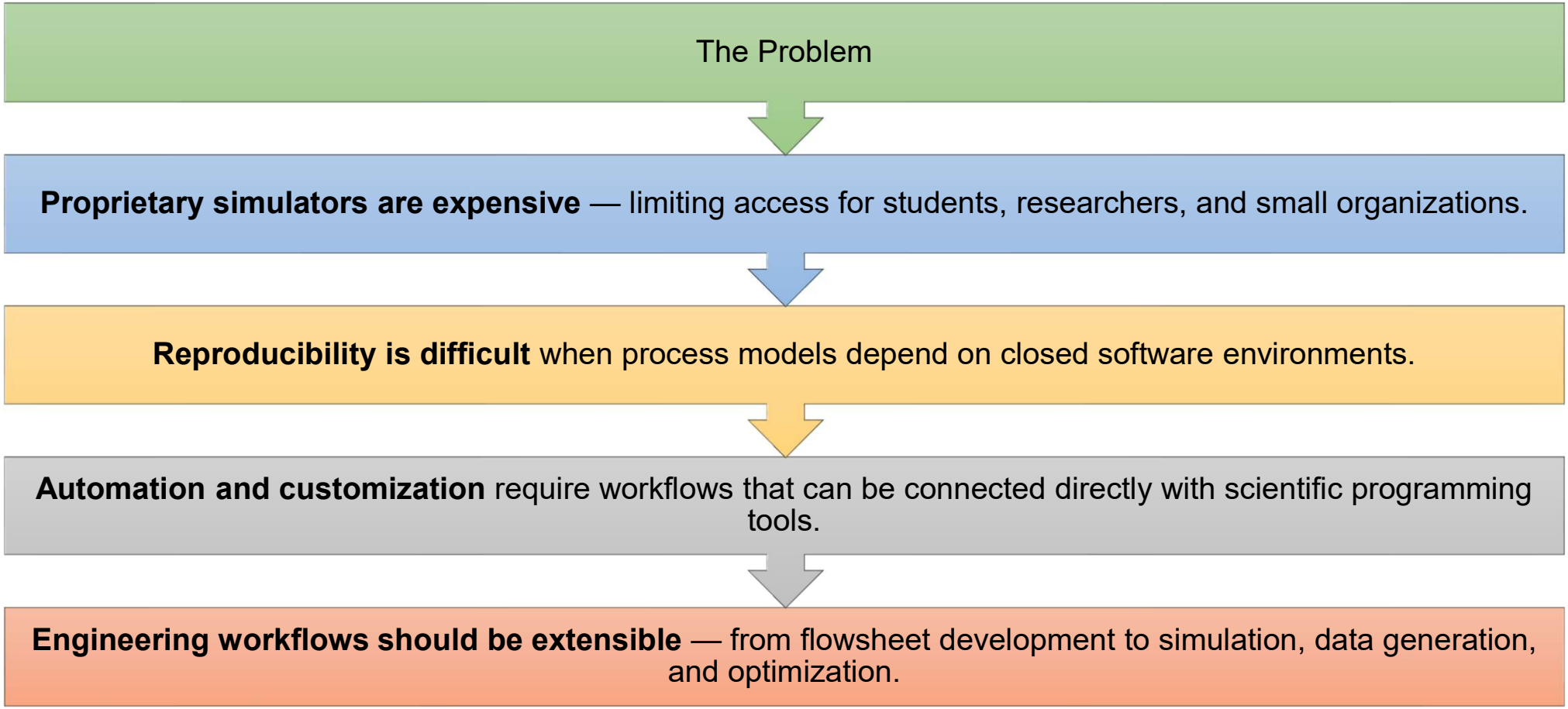
Dr. Sujoy K Samanta
Waste Water Treatment, Microwave Assisted Processing, Renewable Energy

Dr. Sushant Kumar
Heterogeneous Catalysis, Operando Spectroscopy, Clean Energy

Dr. Ganesh Swain
Bioremediation of Wastewater, Bioenergy, Membrane Development

Dr. Sonal Shrivastava
Kinetic modelling,Reaction engineering,Fischer Tropsch Synthesis

Why Open-Source Process Simulation?



Why Process Simulation?

- From Process Concept to Operating Strategy

1. Understand Process Behaviour

- Predict how **temperature, pressure, flowrate and composition** affect the process.
- Evaluate interactions between connected process units.

2. Evaluate Process Alternatives

- Compare different **flowsheet configurations and operating conditions** before implementation.
- Examine process performance under different scenarios.

3. Design & Size Equipment

- Estimate required **heat duties, pressure changes, flow conditions and equipment performance**.
- Test equipment specifications under expected operating conditions.

4. Identify Operating Limits

- Study the effect of changing feed and operating conditions.
- Detect conditions that may cause **poor separation, inadequate heat transfer or equipment constraints**.

5. Support Optimization

- Generate a consistent basis for comparing operating strategies.
- Find operating conditions that meet **process objectives and constraints**.

Process simulation allows engineers to test, understand and improve a process before making changes to the real plant.

Aspen Plus: Established Process Simulation Platform

Why Aspen Plus?

- Widely used for chemical process simulation, design and analysis
- Provides rigorous thermodynamic models for process calculations
- Large library of unit operation models for building industrial flowsheets
- Supports material and energy balance calculations
- Used for process design, equipment analysis and optimization
- Provides a mature environment for modelling complex chemical processes

Aspen Plus

This established approach to process simulation can also be implemented through open-source platforms such as DWSIM

DWSIM: An Open-Source Chemical Process Simulator

❑What Does DWSIM Provide?

THERMODYNAMICS

❑***Calculate fluid properties and phase behaviour***
- Peng–Robinson, PRSV2, SRK
- NRTL, UNIQUAC, Wilson, UNIFAC
- Steam tables & CoolProp
- Petroleum characterization

UNIT OPERATIONS

❑***Build realistic process flowsheets***
- 35+ unit operations
- Distillation columns
- Heat exchangers, compressors, pumps, turbines & valves
- CSTR, PFR & equilibrium reactors
- Pipes, controllers & logical blocks

SIMULATION MODES

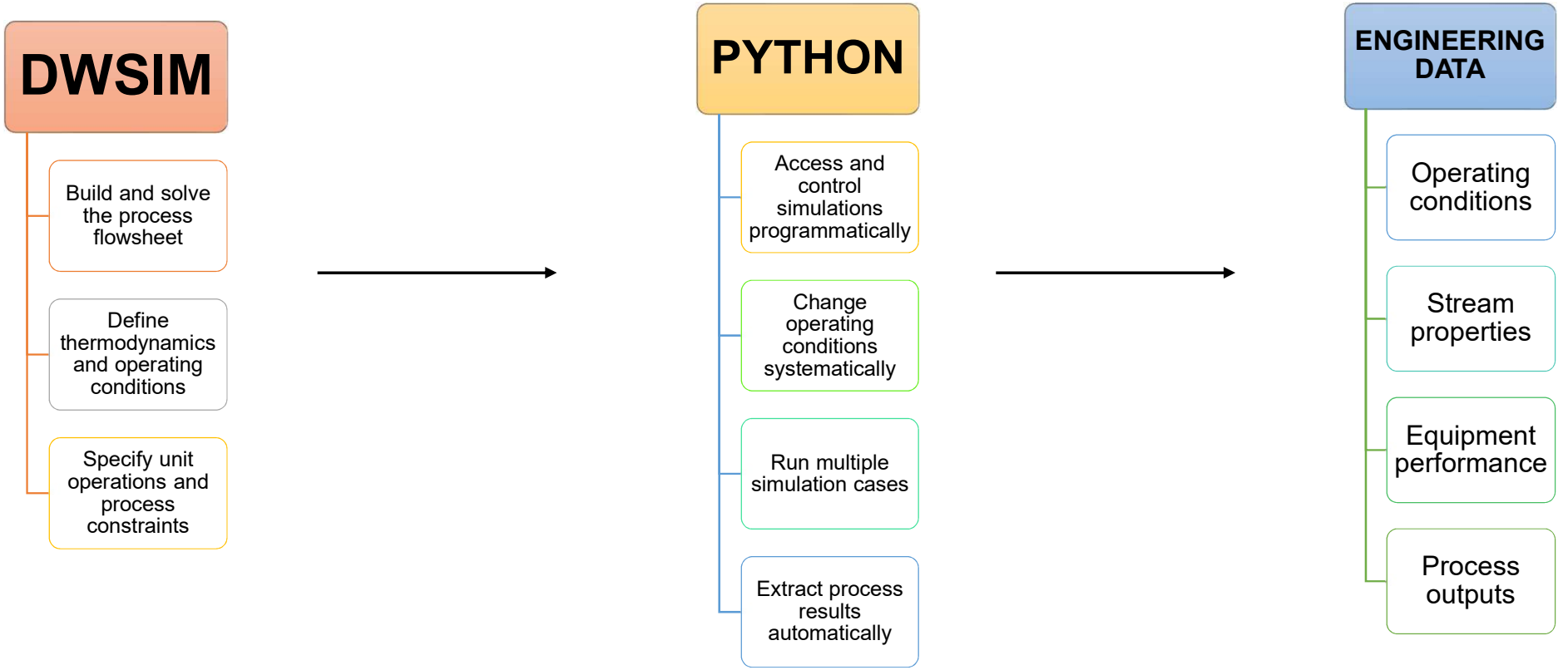
❑***Study process behaviour***
- Steady-state
- Dynamic
- Rigorous time-stepping, controllers & event scheduling

DWSIM
Chemical Process Simulator

DWSIM brings thermodynamics, equipment models and process simulation together in one open-source environment.

DWSIM + Python: From Simulation to Automation

- Move from Manual Cases to a Programmable Workflow



Automated Simulation & Dataset Generation

- Simulation Automation with Python

DEFINE	SIMULATE	GENERATE
• Select key operating variables • Set input ranges and simulation cases • Establish the required process outputs	• Update DWSIM operating conditions • Run simulations through Python • Repeat for multiple operating cases • Collect simulation results	• Organize inputs and outputs • Build a structured engineering dataset • Prepare data for sensitivity analysis and optimization

Python turns a single DWSIM model into a systematic simulation and data-generation workflow.

Sensitivity Analysis & Optimization

- Understanding Process Behaviour

SENSITIVITY ANALYSIS

Vary selected operating conditions systematically

Observe their effect on key process outputs

Identify the variables with the strongest influence

Detect operating regions that require closer attention

OPTIMIZATION

Define process objectives and constraints

Use simulation results to evaluate alternatives

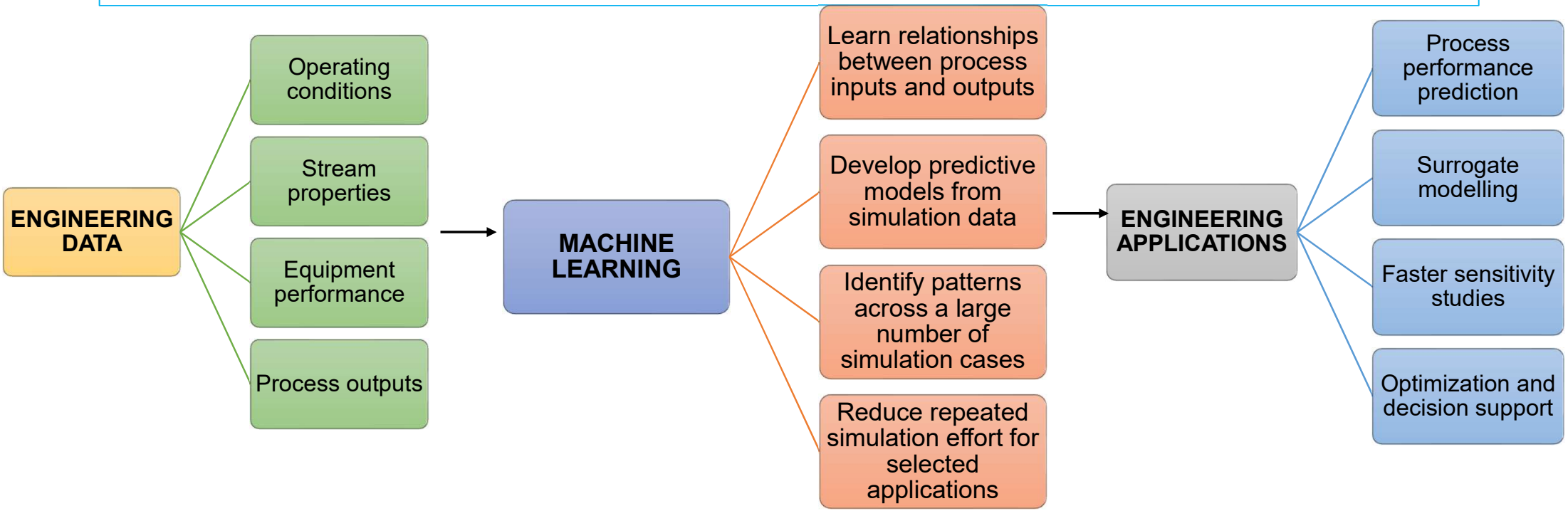
Compare operating conditions and process performance

Identify improved operating strategies

Systematic simulation turns process understanding into informed engineering decisions.

Simulation Data - Machine Learning & AI

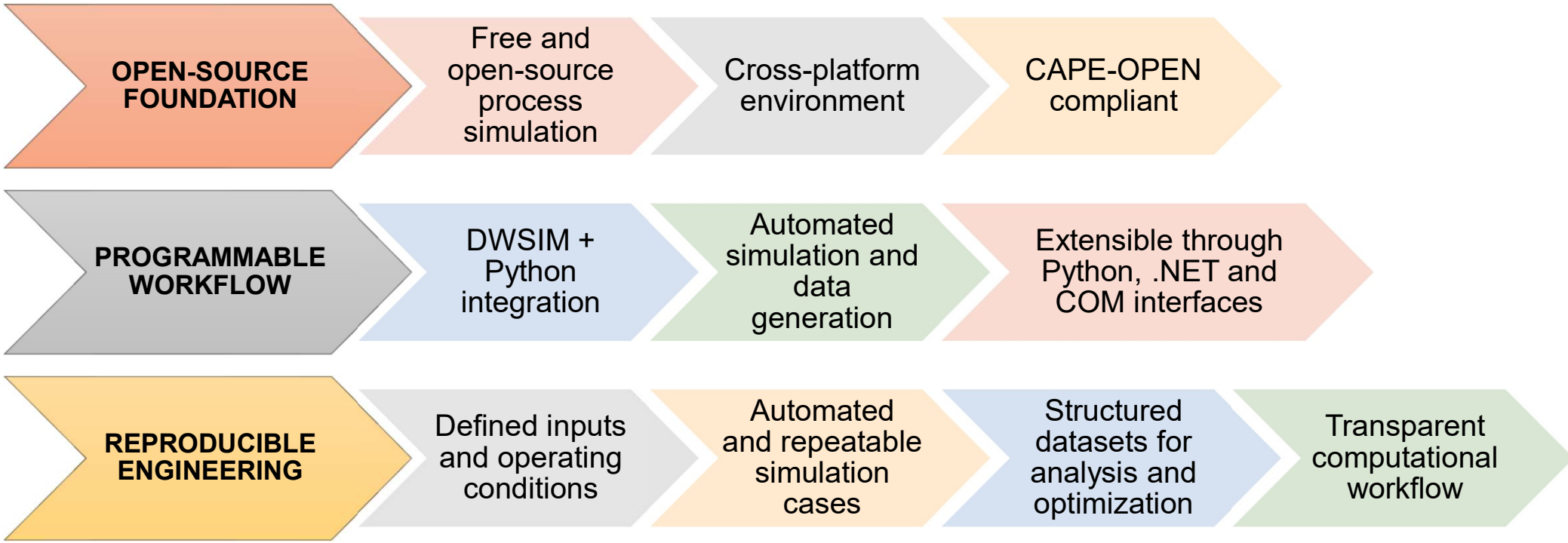
- Turning Engineering Data into Predictive Models



DWSIM provides the engineering data; machine learning provides a data-driven layer for process analysis and optimization.

Reproducible Open-Source Engineering Workflow

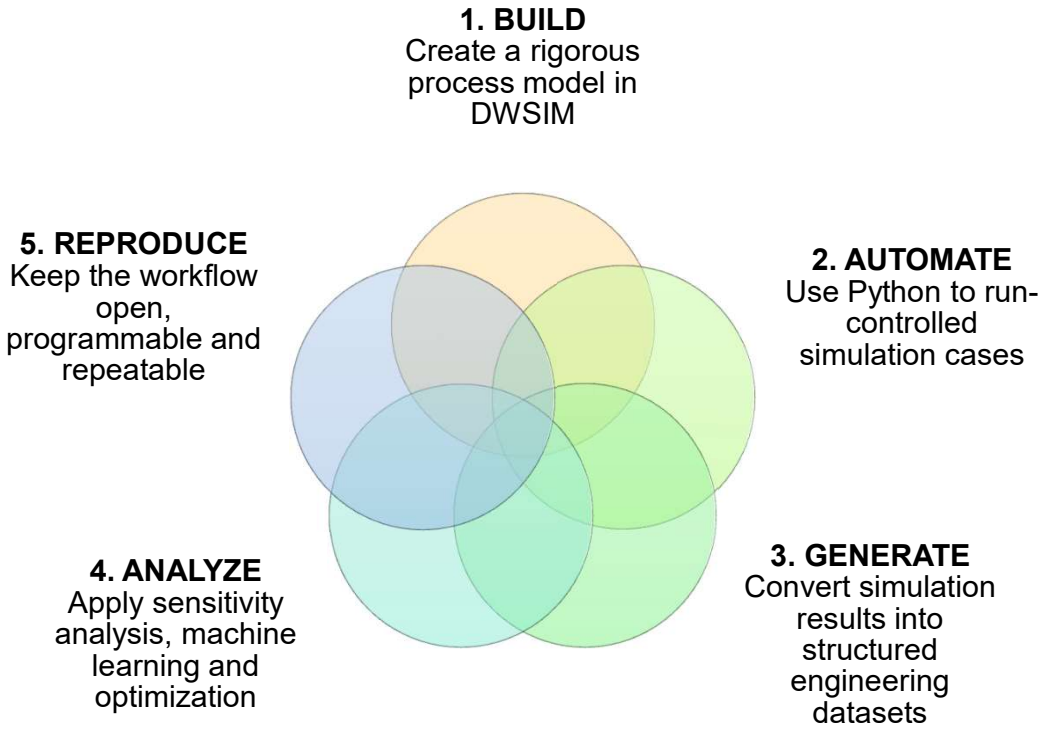
- From Process Simulation to Scalable Engineering



Open-source simulation + programmable automation = reproducible and extensible engineering workflows.

From Flowsheet to Engineering Decisions

- From Flowsheet to AI



Conclusion

- **DWSIM** provides rigorous process simulation in an open-source environment.
- **Python** enables automated and repeatable simulation workflows.
- Multiple simulation cases can be converted into structured engineering datasets.
- These datasets support sensitivity analysis, machine learning and optimization.
- The complete workflow remains open, programmable and reproducible.

Example: Hydrogen Production from Biogas

Process Objective

Produce high-purity hydrogen from biogas through reforming, water-gas shift and PSA separation.

Process Route

Biogas + Steam Reforming
HT-WGS
LT-WGS
Cooling
PSA
H_2 Product

Operating Conditions

- Biogas: **38.5 kg/h**
- Steam: **46 kg/h**
- Reforming: **909°C, 16 bar**
- Methane conversion: **80%**
- HT-WGS: **350°C, 16 bar**
- CO conversion: **75%**
- LT-WGS: additional **75% CO conversion**

Simulation Result

- **H_2 purity: 99.99%**
- **H_2 separation yield: 79%**
- Hydrogen compressed to **350–700 bar** for storage/use.

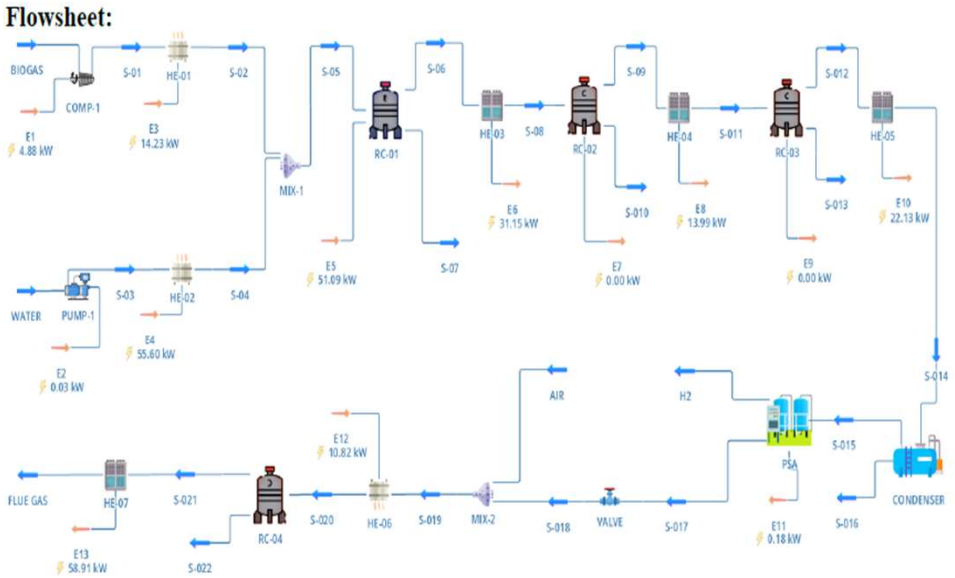


Fig-DWSIM flowsheet for hydrogen production from biogas (H_2-REF process), including biogas reforming, HT-WGS, LT-WGS, PSA separation and tail-gas combustion.

Reference: Phan et al. (2022), International Journal of Hydrogen Energy.

That’s all for now –

✉Contact: nitind@iitp.ac.in

Keep questioning, keep improving, and keep optimizing — in your work, your research, and your life.
Thank you and best wishes for your journey ahead!