Patent Claims

May 12, 2025

1 Introduction

✗ What You Are Not Claiming

1. **Specific Prompt Wording**:
   - The method uses prompts, but we **do not claim** ownership of the **wording** or **the idea of using prompts** in general.
2. **General Use of LLMs**:
   - We **do not claim** the **LLM itself**, or its generic usage, only **how** it is used **in our novel pipeline**.
3. **Generic Reward Model Concept**:
   - We **do not claim** the **concept of reward models** themselves, only **our specific reward application**, combining **multi-metric scoring** and **threshold-based filtering** for **domain-specific dataset generation**.
4. **General Document Retrieval or Clustering**:
   - We **do not claim** retrieval or clustering in isolation, but **only as part of our structured generation pipeline**.
5. We **do not claim** Fine-tuned Models or their deployment — we disclaim ownership over the resulting fine-tuned models or their usage.
6. **We anchor our claims in the specific, integrated, technical pipeline that leverages these known elements in a novel way. What Are we Claiming For : The Method : An automated pipeline for generating, validating, and storing domain-specific synthetic datasets for PFD/PID interpretation and generation, not the models or prompts themselves**

Independent Claim

A computer-implemented method for automated generation, validation, and organization of synthetic instruction–response pairs tailored for fine-tuning domain-specialized small-scale language models in process flow diagram (PFD) and piping and instrumentation diagram (PID) interpretation, analysis, and generation for novel chemicals, the method comprising:

1. receiving, via a data ingestion module, a seed dataset comprising human-authored instruction–response or preference pairs representative of domain-specific chemical process tasks;

2. invoking a pre-existing large-scale language model (LLM) as a generation engine—**explicitly disclaiming any claim of ownership over the LLM architecture, its training data, underlying generation algorithms, and the structure, wording, or phrasing of prompt templates used in the generation process**—to generate multiple types of synthetic instruction–response pairs through recursive conditioning on the seed dataset, the generated synthetic instruction–response pairs including:

   (a) **Factual instruction–response pairs** capturing domain-specific factual knowledge in chemical process engineering to provide the foundational domain knowledge to small-scale language model's;

   (b) **Direct Preference Optimization (DPO) instruction–response pairs** comprising paired candidate responses labeled as preferred and dispreferred, focusing on aligning the small-scale language model's preferences toward more helpful, correct, and contextually appropriate responses. It refines the small-scale language model's response behavior by training it to prefer higher-quality responses over lower-quality resonse;

   (c) **SynDIP instruction–response pairs** comprising structured process context (including background of the process, operational overview, engineering rationale, chemical reactions, reaction mechanisms, and descriptions of unit operations, materials, and flows), along with corresponding sequentially generated PFD textual descriptions and PID textual descriptions;

   (d) **LogiCore instruction–response pairs** comprising multi-step reasoning with explicit chain-of-thought explanations capturing procedural, logical, and engineering reasoning steps for analyzing or justifying PFDs and PIDs;

   (e) **Retrieval-Augmented Instruction-Tuning (RAIT) instruction–response pairs** comprising:

      - **Local RAIT** instruction–response pairs grounded in semantically coherent intra-document content chunks; and

- **Global RAIT** instruction–response pairs grounded in cross-document semantic clusters supporting multi-source reasoning and synthesis;
- "Documents" here refer to external technical knowledge sources, typically engineering documents.

3. evaluating the generated synthetic instruction–response pairs using a configurable multi-metric reward evaluation engine—**explicitly disclaiming any claim of ownership over the reward model architecture, scoring functions, or underlying algorithms**—by applying a weighted combination of predefined quality metrics including helpfulness, factual correctness, logical coherence, response complexity, and verbosity;

4. computing a preference gap for DPO instruction–response pairs by comparing reward scores between preferred and dispreferred responses and filtering based on a predefined preference threshold;

5. grounding the synthetic instruction–response pairs in external document-derived context by:

    (a) retrieving and parsing domain-specific technical content from structured or unstructured knowledge sources;

    (b) clustering the retrieved content into semantically similar groups using vector-based similarity computations to form knowledge clusters for Local and Global RAIT;

    (c) generating multi-scale, context-grounded responses including both brief factual outputs and detailed explanatory outputs;

6. applying predefined quality thresholds to retain only validated synthetic instruction–response pairs meeting or exceeding metrics for factual alignment, coherence, and contextual relevance;

7. storing the reward-validated synthetic instruction–response pairs in a structured digital repository for use in fine-tuning computationally efficient, domain-specialized small-scale language models—**explicitly disclaiming any claim of ownership over the fine-tuned models or their deployment mechanisms**.

Dataset Dependency Structure and Purpose

SynDIP is central as it represents the kind of output the final small language model (SLM) is intended to produce.

Factual QA and **DPO** are more general domain-specific training datasets designed for:

- **Factual QA:** Providing foundational domain knowledge.

- **DPO:** Aligning the model's response preferences toward helpful, correct, and contextually appropriate outputs.

LogiCore, **Local RAIT**, and **Global RAIT** are all derived from or utilize SynDIP content as their primary context. These datasets train the SLM on different aspects of understanding and leveraging detailed process descriptions:

- **LogiCore:** Enabling reasoning about the content.
- **Local RAIT:** Grounding answers in specific, small pieces of the content.
- **Global RAIT:** Synthesizing answers from broader, potentially distributed pieces of related content.

All these datasets are created using teacher LLMs and validated using the **Nemotron-4-340B reward model**, ensuring a consistent quality standard and a unified generation methodology. The overall goal is to train smaller, specialized SLMs to **interpret, analyze, and generate PFDs and PIDs** with high fidelity and adherence to **engineering principles**.

Novelty, Inventiveness, and Technical Contribution

Novelty

The proposed invention introduces a **novel, unified, and automated pipeline** for generating **reward-validated synthetic instruction–response datasets** specifically for **process flow diagram (PFD)** and **piping and instrumentation diagram (PID)** interpretation, analysis, and generation.

This pipeline uniquely integrates:

- Five structured dataset types: **Factual QA**, **DPO**, **SynDIP**, **LogiCore**, and **RAIT (Local and Global)**;
- A **multi-metric reward-based filtering** process;
- A **hierarchically dependent dataset design**, where advanced datasets (LogiCore, RAIT) are **derived from the SynDIP dataset** as the primary context.

No known prior system describes this **specific combination**, **hierarchical dependency**, and **structured pipeline** aimed at **domain-specific small language model fine-tuning** for chemical process engineering tasks.

Inventiveness (Non-Obviousness)

The invention achieves **non-obviousness** through a **curriculum-style, dependency-aware dataset generation strategy**, which:

- **Anchors all advanced tasks** (reasoning, retrieval, synthesis) in a **single primary process flow and instrumentation descriptions** (SynDIP dataset), unlike flat or independent data generation methods;
- **Integrates reward-based preference optimization (DPO)** with **self-instruct synthetic data bootstrapping**, forming a **closed-loop learning pipeline**;
- **Combines document-grounded retrieval (RAIT)** with **multi-scale response generation** and **semantic clustering across documents**, supporting both **localized and globalized contextual grounding**;
- **Orchestrates different learning objectives** (factuality, alignment, reasoning, grounding) into a **hierarchically structured pipeline** that **progressively builds model capabilities**.
- **Purposeful Design of Diverse Synthetic Subsets (Factual QA, SynDIP, LogiCore, DPO, RAIT) to Elicit Specific Engineering Capabilities:** It's not just generating "more data." The non-obvious aspect is the deliberate design and generation of distinct categories of

synthetic QA pairs (Factual QA for foundational knowledge, SynDIP for schematic descriptions, LogiCore for multi-step reasoning, DPO for preference, RAIT for contextual grounding) each tailored to instill a specific, complementary capability required for PFD/PID understanding and generation in SLMs. A person skilled in the art (POSITA) might augment data, but this structured, multi-faceted approach to teaching diverse engineering-relevant skills through targeted synthetic data types is inventive, is a non-trivial conceptual leap.

These elements, when combined, go **beyond obvious extensions** of individual techniques and represent a **non-trivial architectural and methodological advancement**. Inventiveness is in the clever, non-obvious way these specific techniques are combined and adapted within an iterative loop to generate diverse, high-quality synthetic datasets for the specific and challenging domain of chemical PFDs/PIDs.

Technical Contribution

The invention delivers the following **technical contributions**: Technical Contribution is the practical, measurable improvement this pipeline offers: a scalable way to get better training data, which leads to better-performing and more efficient AI models for a specialized industrial application. The pipeline provides a concrete, automatable, and systematic method for producing large volumes of diverse, high-quality synthetic datasets tailored for chemical process engineering (PFDs/PIDs). This has practical implications for deployability and resource consumption. This directly addresses the bottleneck of insufficient, expensive, or inconsistently human-annotated data in this specialized domain. By providing high-quality synthetic data, the pipeline facilitates the fine-tuning of smaller, more efficient small-scale language models(SLMs) to perform complex chemical engineering tasks that might otherwise require much larger models or significant human expertise.

1. **Automated Generation of Domain-Specialized Training Data:** Reduces reliance on costly human annotation by using **reward-validated synthetic data pipelines**.

2. **Hierarchical, Context-Consistent Dataset Structuring:** Ensures **internal consistency and reuse** by **deriving advanced reasoning and retrieval tasks from a single process flow and instrumentation descriptions**, improving learning alignment.

3. **Multi-Metric Reward Filtering with Preference Gap Enforcement:** Enhances **quality control and model alignment** using **weighted multi-objective evaluation** and **preference gap scoring**.

4. **Retrieval-Augmented, Multi-Scale Answer Generation:** Improves **factual grounding and scalability** by combining **document retrieval, semantic clustering**, and **layered response generation** (short/long).

5. **Practical Impact on Small-Scale Model Deployment:** Enables **cost-effective, accurate, and specialized model deployment** for **chemical process engineering applications**, including **PFD and PID generation**.