Patent Claims

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May 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:

- receiving, via a data ingestion module, a seed dataset comprising humanauthored instruction—response or preference pairs representative of domainspecific 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 crossdocument 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.