HYDROCARBON PROCESSING®

Originally appeared in
Hydrocarbon Processing, September 2025.
Posted with permission.

SPECIAL FOCUS: REFINING TECHNOLOGIES

AI-/ML-based hybrid modeling for enhanced resid fluid catalytic cracking optimization

F. M. AL JABERI, M. AL MUSHARFY, B. SAHA, A. TAHER, A. M. ALSUWAIDI, M. AL BLOOSHI, S. MANTRIPRAGADA, V. S. THAMIZHA and **R. D. POLONIA,** ADNOC, Abu Dhabi, United Arab Emirates; and **D. PERIYASAMY, P. JAIN** and **S. SHEIKH,** Emerson's Aspen Technology business, Abu Dhabi, United Arab Emirates

This article discusses the development and deployment of an artificial intelligence (AI)-/machine-learning (ML)-based hybrid model to improve prediction accuracy in resid fluid catalytic cracking (RFCC) processes. By combining first principles-based modeling with data-driven ML algorithms, the hybrid model overcomes limitations of traditional linear programming (LP) sub-models. Results showed significant accuracy improvements, reduced yield variances and better operational flexibility, leading to notable economic benefits for refinery planning and optimization.

Limitations. Refinery planning has long been reliant on LP models, which are integral to decision-making processes like yield prediction and economic optimization. However, the limitations of LP sub-models, particularly in handling nonlinear process behaviors and operating variability, often lead to inaccuracies and sub-optimal plans. Frequent updates to yield predictions and manual LP vector adjustments further complicate operations, introducing inefficiencies.

Rigorous simulation models are very accurate, very complex models with tens of thousands of variables and thousands of equations, making them too heavy for a multi-site level optimization solution that covers the full value chain like planning models.

To address these challenges, ADNOC Refining has developed a high-fidelity AI-/ML-based hybrid model for RFCC processes using a hydrid model[a]. This model combines the strengths of first principles-based modeling with ML techniques, capturing nonlinear process dynamics and enhancing predictive capabilities across a broader range of operating conditions.

Moreover, the hydrid model developed for this project is as accurate as that of the co-author's company's rigorous process models[b] in the defined wider operating envelope, and it needs very low computational needs vs. an LP model.

Challenges in refinery planning. Refinery planning faces several challenges due to the limitations of traditional LP models. Key challenges include:

- **Limited validity of LP models:** Traditional LP sub-models fail to maintain accuracy over wider operating ranges, necessitating frequent updates (**FIG. 1**).
- **Variance in product properties:** Traditional LP models assume constant properties for the whole swing cut. When part of the swing cut is added to the adjusting lighter and heavier

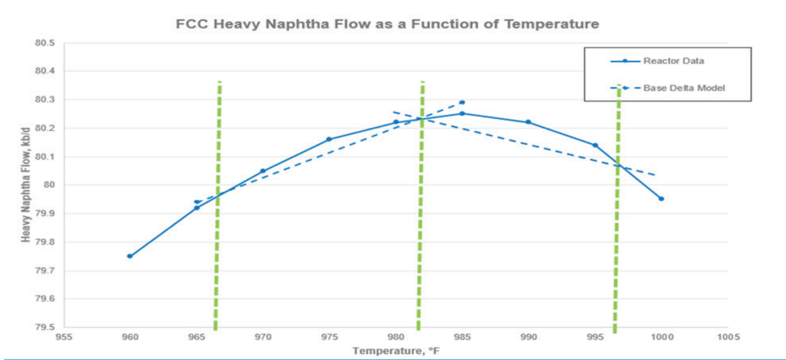

FIG. 1. Linearization of non-linear process behavior.

products, the same swing-cut properties are used for blending calculations to arrive at the properties of lighter and heavier cuts (**FIG. 2**). These approximation errors in swing-cut properties and blending calculations lead to deviations in product qualities.

- **Sub-optimal plans:** Inaccuracies in LP models result in non-optimal operational and economic outcomes.
- **Manual workflow complexity:** Non-standard workflows for LP vector generation contribute to inefficiencies. In addition, LP models are accurate only in a very narrow range of operating conditions. A major shift in operating conditions necessitates LP vector generation for the new operating regions.

Hybrid modeling overview. Hybrid models combine the intelligence of AI with the domain experience of engineering first principles to deliver a comprehensive, accurate, fit-for-purpose model. This approach retains the physical and chemical understanding of the process while leveraging data-driven insights to address gaps in traditional models. The result is a robust predictive framework suitable for extrapolation and broader applicability.

The AI/ML-based hybrid model developed by ADNOC Refining demonstrates the following advantages:

- Enhanced prediction accuracy
- Reduced dependency on manual updates
- Improved adaptability to varying operating conditions.

Methodology. The foundation of the hybrid model lies in a calibrated RFCC process model[b] (**FIG. 3**). Key features include:

- **Two regenerators and two risers:** Parallel configurations with extended kinetics for light-end predictions, such as propylene yield.
- **Downstream modeling:** The incorporation of short-cut columns to capture downstream dynamics.

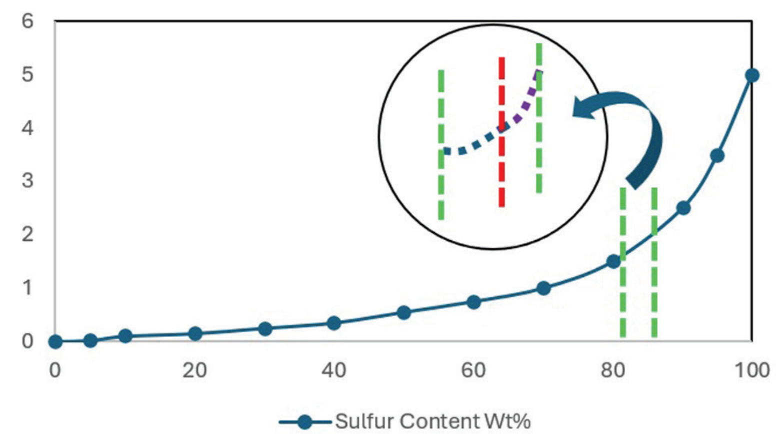

FIG. 2. Assumption of constant property for the whole swing-cut.

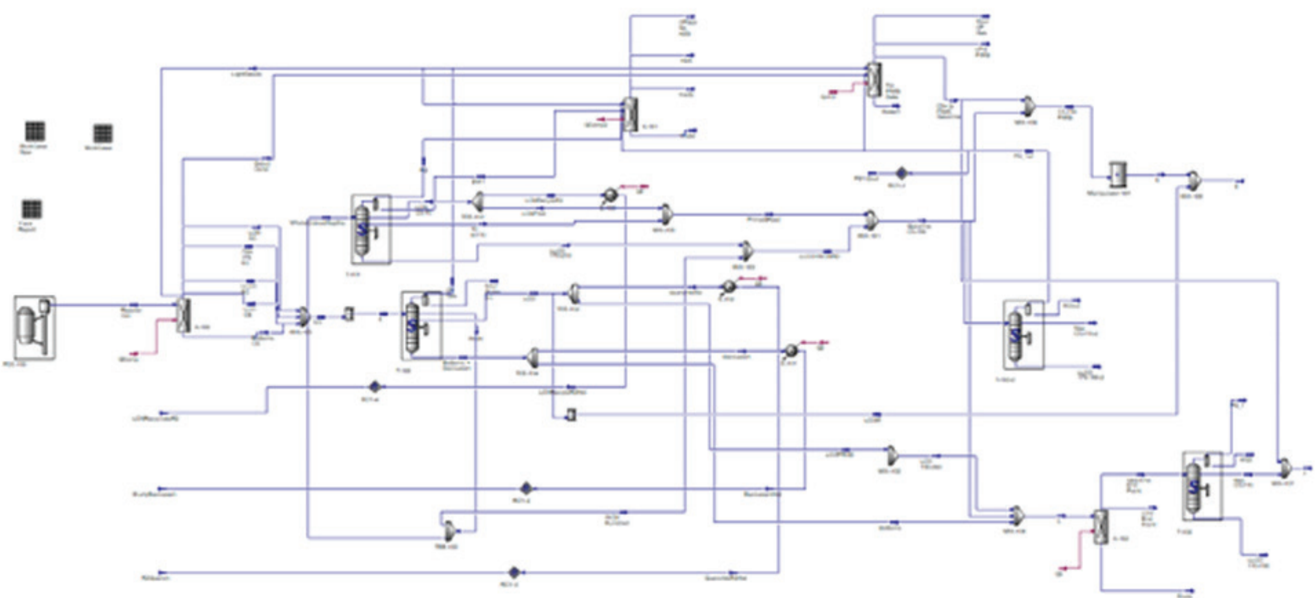

FIG. 3. Flowsheet of an RFCCU in the co-author's process model[b].

The RFCC model was calibrated using a set of test-run data and validated through cross-prediction against five different data sets across wider operating ranges to ensure model accuracy.

Data generation and model building. The hybrid model development followed a systematic workflow:

1. **Data generation:** The process model[b] was run within the co-authors' company's multi-case program[c], where the independent and dependent variables were selected based on the planning model structure. Lower and higher bounds for each independent variable were defined based on the operating window of the RFCCU. The multi-case program[c] generated 1,653 case study results, covering the full operational envelope.
2. **Hybrid model[a] creation:** The results from the multi-case program[c] were used to develop a reduced order hybrid model with first-principle constraints in an AI model builder. The hybrid models developed through this method are fit-for-purpose models that meet the planning model requirements and produce results that are comparable to the rigorous process models[b] within the set operating limits, ensuring accurate representation of RFCCU behavior (**FIG. 4**).
3. **Hybrid model[a] validation:** Parity plots, R2 and Q2 plots were employed to validate the model's accuracy and predictability. In addition, co-efficient plots that provide insights into the dependencies among the variables were analyzed to validate if the hybrid model reflects actual behavior in the plant.

Hybrid model[b] deployment. The hybrid model was imported as an external sub-model into a proprietary planning system[d], where it was integrated with refinery planning workflows. The deployment was completed with the following steps to ensure proper integration and validation:

- Standalone planning system[d] model response testing
- Cross-prediction against multiple datasets
- Back-casting for accuracy verification.

Results and benefits. The following is a comparison of base delta vs. the hybrid model vs. actual plant data. The deployment of the hybrid model resulted in significant improvements:

- **Improved accuracy:** The hybrid model outperformed traditional base-delta models, providing a better fit with plant data. The deployment of the hybrid model resulted in significant improvements against the LP model, as shown in **FIG. 5** and **TABLE 1.**
- **Yield variance reduction:** With the integration of the RFCC hybrid model, the yield variance (plan vs. actual) was reduced in many product pools.
- **Operational flexibility:** The model's adaptability to broader operating ranges decreased the frequency of model updates.
- **Economic gains:** Retro-optimization revealed further margin improvements, contingent on relaxation of certain process constraints. The retro-optimization showed the following changes in the product pools:
  - **Middle distillate:** Increased 1%
  - **Gasoline:** Increased 3%
  - **Propylene:** Increased 7%
  - **Excess slurry:** Decreased 9%.
- **Operational flexibility:** The model's adaptability to broader operating ranges decreased the frequency of process industry modeling system (PIMS) updates.

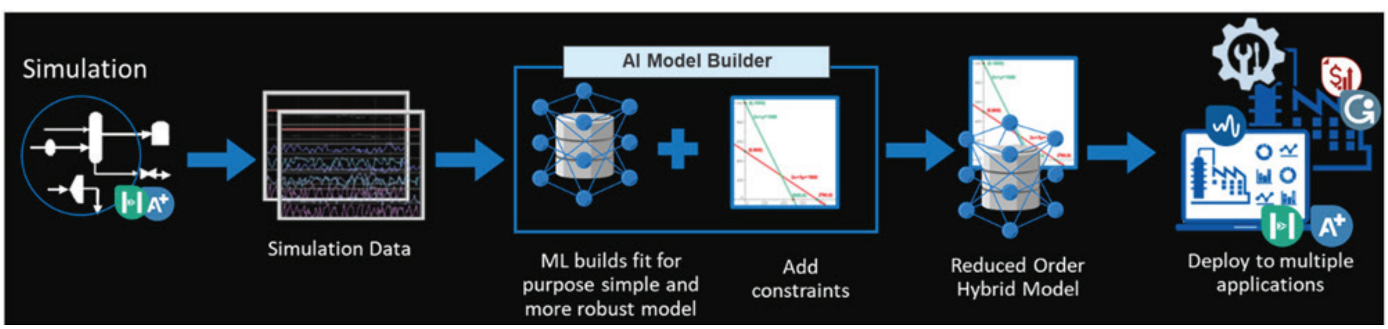

FIG. 4. Workflow for hybrid model data generation and creation.

Learnings and best practices. The adoption of hybrid modeling has underscored several best practices:

- Utilize calibrated models with comprehensive datasets for robust hybrid model development.
- Incorporate rigorous validation techniques (e.g., R2 and Q2 metrics) to ensure model reliability.
- Foster interdisciplinaary collaboration between domain experts and data scientists to enhance model accuracy.

Takeaway. The AI-/ML-based hybrid model represents a significant advancement in refinery planning, addressing the limitations of traditional LP sub-models. By combining first principles and ML approaches, the model achieved higher accuracy, operational flexibility and economic optimization. This innovative framework has demonstrated an improved business process for planning model updates and improved refining margins by driving the plan towards true optimum. The hybrid models have the potential to redefine process modeling and optimization in the refining industry. **HP**

ACKNOWLEDGMENTS

The authors express gratitude to ADNOC Refining for supporting this initiative and providing the necessary resources and insights about RFCC and planning workflows at ADNOC Refining, as well as AspenTech for providing the expertise on model development, deployment and validation.

ADNOC STATEMENT

© 2025 ADNOC Refining. All rights reserved. The technical innovations, methodologies and results presented are protected by trade secrets, copyright and potential patent rights. No part of this work may be reproduced, adapted or implemented commercially without express written permission from ADNOC Refining.

NOTES

a Aspen HYBRID models
b Aspen HYSYS
c Aspen Multi-Case™
d PIMS-AO

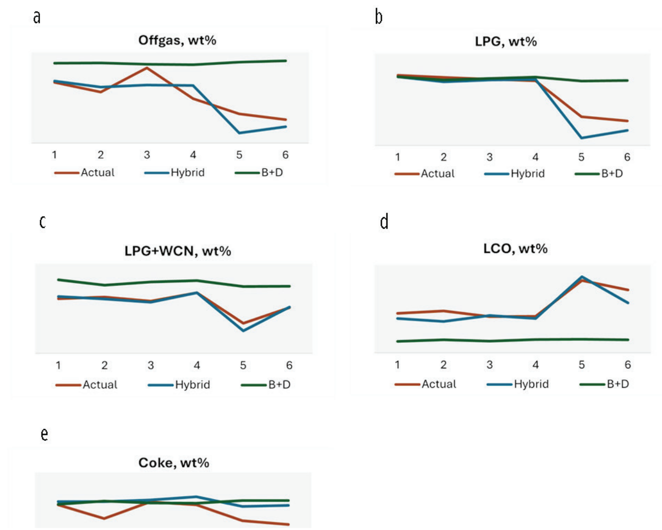

FIG. 5. The deployment of the hybrid model resulted in significant improvements against the LP model.

TABLE 1. Comparison of the models

RFCC % error	Hybrid	B + D
Data set 1	5.2%	12.1%
Data set 2	6.4%	12.3%
Data set 3	4.8%	11.6%
Data set 4	2.1%	6.4%
Data set 5	8.2%	16.5%
Data set 6	9%	16.1%
Average across all sets	5.9%	12.5%

Article copyright © 2025 by Gulf Energy Information. All rights reserved. Printed in the US.
Not to be distributed in electronic or printed form, or posted on a website,
without express written permission of copyright holder.