CHEMICAL ENGINEERING TRANSACTIONS
VOL. 119, 2025
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it
Guest Editors: David Bogle, Flavio Manenti, Piero Salatino

ISBN 979-12-81206-20-5; **ISSN** 2283-9216
DOI: 10.3303/CET25119093

Optimization of Catalytic Methane Oxidation Using Hybrid Gaussian Process and Fisher Information-Based Experimental Design Strategies

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Gaussian Process (GP) modelling has gained momentum as a powerful data-driven technique for effectively modelling and optimizing complex reactor systems due to its ability to predict nonlinear behaviours and quantify prediction uncertainty. In the context of optimal experimental design, Fisher Information Matrix (FIM) is a common metric used to quantify how sensitive the response of a reaction system is with respect to its kinetic model parameters and to quantify the prediction uncertainty in mechanistic models. The focus of this research is to understand how key performance indicators (KPIs) of a reaction system are influenced by the information content of the experimental design space as quantified by FIM metrics. To achieve this, a hybrid technique that combines mechanistic modelling with data-driven GP modelling was developed, where a first GP (GP1) is used to map the relationship between the FIM and KPIs and a second GP (GP2) is used to model the relationship between operating conditions and FIM using actual lab data. The approach was tested on a case study of complete methane oxidation, showing a clear positive correlation between high values of FIM metric and high conversion of reactant – the main KPI considered in this study.

1. Introduction

Methane oxidation plays an important role in the process industry and has been pivotal in helping to reduce greenhouse emissions, pollution control, and natural gas combustion (Karakurt et al., 2012). Despite its importance, optimizing methane reaction has been a difficult one owing to the nonlinearity of its kinetic dynamics, uncertainties in its kinetic models, and high cost of running the experiments (Tao et al., 2018). Data-driven methods such as Gaussian Processes (GPs) have emerged as a useful tool for modelling complex reactor systems by predicting their nonlinear behaviour and quantifying prediction uncertainty (Abdar et al., 2011). Similarly, Model-based Design of Experiments (MBDoE) approaches leverage Fisher Information Matrix (FIM) metrics by quantifying parameters sensitivities to aid optimal experimental design and minimise prediction uncertainty (Cenci et al., 2023). MBDoE methods identify the most informative regions of the experimental design space for parameter estimation (Friso and Galvanin 2024), thereby improving model identifiability and reliability. Both GP-based and MBDoE approaches have been successfully applied in the design of experiment paradigms. However, their combined potential to link information content (measured by FIM) with key performance indicators (KPIs) in reaction systems, such as conversion, selectivity, and yield, remains largely unexplored—this is the main gap addressed in this work. GPs are well regarded for their ability to predict nonlinear system behaviours with high accuracy, they typically do not incorporate the mechanistic understanding embedded in traditional kinetic models (Samuel et al., 2024). In contrast, FIM-based methods focus on parameter identifiability but often overlook direct influences of the experimental design variables on system-level KPIs, which are essential for operational and strategic decisions in industry (Yang et al., 2022). Designing experiments that simultaneously improve operational results and model reliability has proven challenging due to different limitations in both approaches (Barad, 2014). For example, when applying these techniques to the reaction of catalytic methane oxidation in flow (Bawa et al., 2023) FIM-driven methods might find optimal experimental conditions that minimize the uncertainties in kinetic parameters, but without giving priority to conditions that maximize methane conversion.

The aim of this study is to account for this limitation in both approaches by developing a hybrid experimental design framework that integrates GP modelling and FIM analysis to optimize the design of experiments in catalytic methane oxidation. The proposed framework correlates the system information (FIM) gain with the operational KPI (methane conversion) to identify trade-off experimental conditions where high information

Paper Received: 27 June 2025; Revised: 20 July 2025; Accepted: 3 October 2025
Please cite this article as: Aku M., Bawa S.G., Lee Y.S., Galvanin F., 2025, Optimization of Catalytic Methane Oxidation Using Hybrid Gaussian Process and Fisher Information-Based Experimental Design Strategies, Chemical Engineering Transactions, 119, 553-558 DOI:10.3303/CET25119093

content aligns with system optimal performance. The hybrid framework makes use of two synergistic GP models: i) a first GP (GP1) to map FIM scores to methane conversion prioritizing informative experiments; ii) a second GP (GP2) inversely links reactor conditions to FIM scores, enabling an inverse design strategy to translate optimal FIM targets into actionable operating conditions. Validation through sequential insilico experiments and real experiments demonstrates how this dual-GP approach reduces experimental costs while improving KPI predictions.

2. Methodology

2.1 Proposed Hybrid Workflow

A schematic for the proposed hybrid workflow combining two Gaussian Processes (GP1 and GP2) and FIM analysis is shown in Figure 1. In the workflow GP1 is a forward GP model that maps the FIM score, a metric of information on mechanistic model parameters, to methane conversion values. This model predicts conversion outcomes and their associated uncertainties, enabling direct validation against experimental or *in* silico data. GP2 is a second forward GP model that links reactor operating conditions (**u**) to FIM scores. Critically, GP2 does not estimate reactor conditions directly; instead, its inversion is used to optimize **u** for target FIM score. Experimental data from 30 actual experimental runs by Bawa et al. (2023) served as the starting point for GP1 and GP2. The six topmost informative experiments based on their FIM scores were used for GP1 while data from the full set of 30 experiments was used for GP2. Both models were trained and validated from the existing data (GP1 with 5-fold cross-validation, and GP2 with a 20% test set) and an R^2 value above 0.8 was used as the stopping criterion in training for both models. An R^2 threshold above 0.8 was selected as it reflects strong model performance, especially in small, noisy experimental datasets where values above 0.9 are often unrealistic (Li et al., 2019). Once trained, GP1 was employed to design the next sequence of experiments and predict conversion and corresponding uncertainties. GP1 is then combined with GP2 in the workflow to determine the reactor conditions for the designed experiments.

Figure 1 describes the integrated workflow where optimized GP1 is inverted to estimate the corresponding FIM score based on its predicted methane conversion. This estimated FIM score then serves as an input to GP2. Using an inverse design strategy, GP2 estimates the corresponding optimal reactor conditions (**u**), and the procedure continues until GP1 prediction of conversion uncertainty falls below a threshold set by the user (here 1%). An additional validation of GP1 conversion is done by conducting in silico experiments to estimate the conversion at the predicted optimal reactor conditions (**u**).

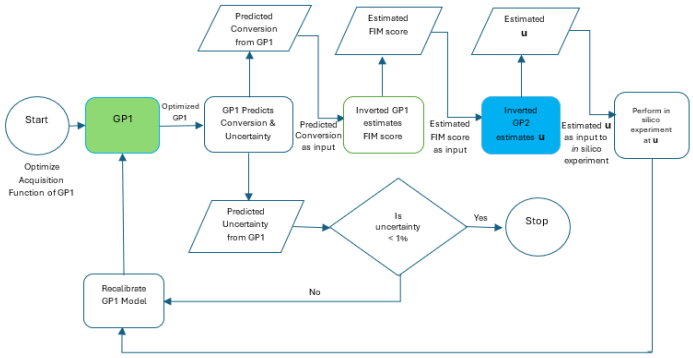


Figure 1: Schematic workflow illustrating the sequential use of GP1 (green box) and GP2 (blue box) models.

The procedure for GP1-GP2 workflow shown in Figure 1 is articulated in the key steps below:

1. Start: an optimization of GP1's acquisition function, whose objective is to optimize methane conversion, is carried out. After the optimization, GP1 is then used to predict and design one experiments at a time until the stopping criterion is met.
2. GP1 Predictions: the optimized GP1 predicts conversion of methane and corresponding uncertainty.
3. GP1 Inversion: GP1 is inverted to estimate the corresponding FIM at the predicted conversion.
4. GP2 Inputs: the estimated FIM score from the inverted GP1 is then used as inputs into the GP2
5. GP2 Inversion: GP2 is inverted to estimate the corresponding reactor condition **u**, based on the inputted FIM score estimated by GP1 inversion.
6. *In* silico Experiment: estimated reactor conditions from GP2 inversion are then used to run computer simulated experiments.

Stopping Criterion: the workflow continues and only stops when the GP1 predicted uncertainty on the KPI falls below 1%. The procedure detailed above has been applied to a gas phase flow reactor model where a reaction of catalytic methane oxidation occurs (Bawa et al., 2023; Pankajakshan et al., 2023). Models used in the mechanistic part of the framework (FIM evaluation) and the data-driven part (GPs) are detailed in the following sections.

2.2 Reactor Model for Methane Oxidation

The methane oxidation system is governed by a set of differential-algebraic equations (DAEs) describing state variables, inputs, and measured outputs:

$$f(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{u}, \boldsymbol{\theta}, t) = 0 \quad (1)$$

$$\mathbf{y} = h(\mathbf{x}, \mathbf{u}, \mathbf{v}) \quad (2)$$

where $\mathbf{x} \in R^{n_x}$ is the vector of state variables, $\dot{\mathbf{x}}$ is their derivative with respect to time t, $\mathbf{u} \in R^{n_u}$ the vector of manipulated input variables, assumed to be time-invariant in this study, and $\boldsymbol{\theta} \in R^{n_\theta}$ the vector of model parameters. The output vector $\mathbf{y} \in R^{n_y}$ denote the vectors of response variables that are measurable (Asprey and Macchietto, 2000) and $\mathbf{v} \in R^{n_v}$ denoted the process or measurement noise. Although the general system formulation in Equations (1) and (2) are expressed with respect to time t, the reactor model employed in this study is defined with respect to catalyst mass w as the independent variable, which is common in plug flow catalytic reactor modelling. The detailed reactor model for catalytic methane oxidation, originally proposed by Bawa et al. (2023) and later adapted by Aku et al. (2025) is expressed through the following system of ordinary differential equations (ODEs) with respect to the catalyst mass *w* (g):

$$\frac{dx_1}{dw} = \frac{R.u_1}{u_2 P_{avg}} - r \;\; x_1(0) = u_4; \;\; \frac{dx_2}{dw} = \frac{R.u_1}{u_2 P_{avg}} - 2r \;\; x_2(0) = u_3.u_4; \quad \frac{dx_3}{dw} = \frac{R.u_1}{u_2 P_{avg}} r; \quad \frac{dx_4}{dw} = \frac{R.u_1}{u_2 P_{avg}} 2r \quad (3)$$

In Equation (3), the vector of state variables is given by $\mathbf{x} = [x_1, x_2, x_3, x_4]^{\mathrm{T}}$, where x_1, x_2, x_3, and $x_4$represent the mole fractions of methane (CH_4), oxygen (O_2), carbon dioxide (CO_2), and water (H_2O), respectively. r represents the rate of reaction [mol g^{-1} s^{-1}], R is the universal gas constant [J mol^{-1} K^{-1}], and P_{avg} is the average pressure inside the reactor [atm]. The vector of control variables $\mathbf{u} = [u_1, u_2, u_3, u_4]^{\mathrm{T}}$ defines the experimental operating conditions, where, u_1 is the reaction temperature T [℃], u_2 the feed flow rate m [Nml min^{-1}], u_3 the oxygen to methane molar ratio R_{O_2/CH_4} [mol mol^{-1}], and u_4 inlet methane mole fraction Y_{CH_4} [mol mol^{-1}]. These controls form the design vector $\boldsymbol{\varphi}$ which is bounded within the experimental design domain as shown in Table 1. The conversion of methane α is defined as the fraction of methane consumed during the catalytic oxidation process over palladium-based catalyst:

$$\alpha = \frac{Y_{CH_4} - y}{Y_{CH_4}} \quad (4)$$

where y is the measured methane concentration in the reactor *effluent (*measured response). The experimental data used in this study was obtained from catalytic methane oxidation tests conducted by Bawa et al. (2023), which involved a packed bed plug flow reactor operating under atmospheric pressure with a Pd/Al_2O_3 catalyst. The experiments were carried out at varying inlet compositions, flow rates, oxygen to methane mole ratio and temperatures ranges as shown in Table 1.

Table 1: Upper and lower bounds on control variables defining the experimental design space.

Control Variables	Range	Unit
Temperatures	250-350	℃
Mass flow rate	20-30	$Nml\ min^{-1}$
Oxygen to methane mole ratio	2-4	$mol\ mol^{-1}$
Methane mole fraction	0.005-0.025	$mol\ mol^{-1}$

2.3 FIM-Based Experiment Ranking

The information content of each candidate experiment is quantified using the Fisher Information Matrix (FIM). For the Mars-van Krevelen (MVK) kinetic model (Pankajakshan et al., 2023), the FIM computed for each set of reactor conditions $I(\boldsymbol{u})$ and the corresponding FIM score $I_{Abs}(u)$ for each experiment are defined by Equation 5 and 6,

$$I(\boldsymbol{u}) = \left(\frac{dy(\boldsymbol{u})}{d\theta}\right)^T \Sigma^{-1} \left(\frac{dy(\boldsymbol{u})}{d\theta}\right) \quad (5)$$

$$I_{Abs}(\boldsymbol{u}) = \text{trace}\ (I(\boldsymbol{u})) \quad (6)$$

where $\frac{dy(\boldsymbol{u})}{d\theta}$ is the sensitivity matrix of output *y* with respect to parameters θ, and Σ^{-1} is the inverse of the covariance matrix, *I* ($\boldsymbol{u}$) is the Fisher Information Matrix (FIM) for condition $\boldsymbol{u}$, $|I\ (\boldsymbol{u})_{i,j}|$ denotes the absolute value of matrix elements respectively. The experiments are then ranked based on their FIM score.

2.4 Gaussian Process Modelling

Gaussian Process (GP) regression applies a non-parametric Bayesian method to model complex relationships between inputs and outputs while quantifying predictive uncertainty. This work employs two distinct GP models:

1. **GP1**. It maps FIM scores to methane conversion. The FIM score for each experiment is calculated from Equation 5, and the methane conversion is obtained from Equation 4. The model incorporates a logit transformation to bound predictions between 0 and 100%. The logit transformation is computed from Equation 7, where α is the conversion of methane. The GP1 function is defined in Equation 7.

$$y_{logit} = \ln\frac{\alpha}{1-\alpha} = GP1(\mu(I_{Abs}), k(I_{Abs}, I_{Abs}{}')) \quad (7)$$

   where y_{logit} is the logit-transformed methane conversion, $\mu(I_{Abs})$ is the mean function of the GP dependent on the FIM score, and $k(I_{Abs}, I_{Abs}{}')$ is the kernel (covariance) function evaluating the similarity between two FIM scores $(I_{Abs}, I_{Abs}{}')$.

2. **GP2**. It maps reactor operating conditions $\mathbf{u}$ to Absolute FIM (I) scores for inverse design. The goal of inverse design process is to find the design variables for a given output target. In this scenario, the GP2 model and the inverse design problem is formulated in Equation 8, and 9 respectively.

$$I_{Abs}(\boldsymbol{u}) = GP2(\mu(\boldsymbol{u}), k(\boldsymbol{u}, \boldsymbol{u}')) \quad (8)$$

$$\boldsymbol{u}^* = \arg\min|GP2(\boldsymbol{u}) - I_{Abs}{}^*| \quad (9)$$

   where $\mu(\boldsymbol{u})$ is mean function of GP2, dependent on reactor conditions ($\boldsymbol{u}$), and $k(\boldsymbol{u}, \boldsymbol{u}')$ is the kernel function evaluating similarity between two reactor conditions sets $(\boldsymbol{u}, \boldsymbol{u}')$.

2.5 Data Preparation and Partitioning for GP1 and GP2 Modelling

For GP1 only the six topmost informative experiments were used; after fine tuning GP1, the acquisition function (Expected Improvement) was optimized to favor high conversion of methane. For GP2, the 30 experimental datasets were split into training (70%), testing (20%), training and validation (10%). Both GP1 and GP2 use the same combination of three kernels to model methane oxidation: (1) a *constant kernel* (fixed signal strength = 1.0), (2) an *RBF kernel* (smoothness scale = 1.0) to capture nonlinear trends, and (3) a *noise kernel* (low noise level = 10^{-6}) for measurement errors. These components were tuned within strict physical limits to ensure accurate predictions without overfitting the data. An additional noise term (for methane response) from the measured experiments by Bawa et al., 2023 was also introduced to the GPs.

3. Results and Discussion

This section discusses the performance and validation of GP1 and GP2. The simulation scenario involves training GP1 on six real experiments to design future experiments by exploring regions of high methane conversion, while evaluating uncertainty and FIM scores. It also covers methane conversion and FIM values based on GP1's predictions, alongside the performance of both models.

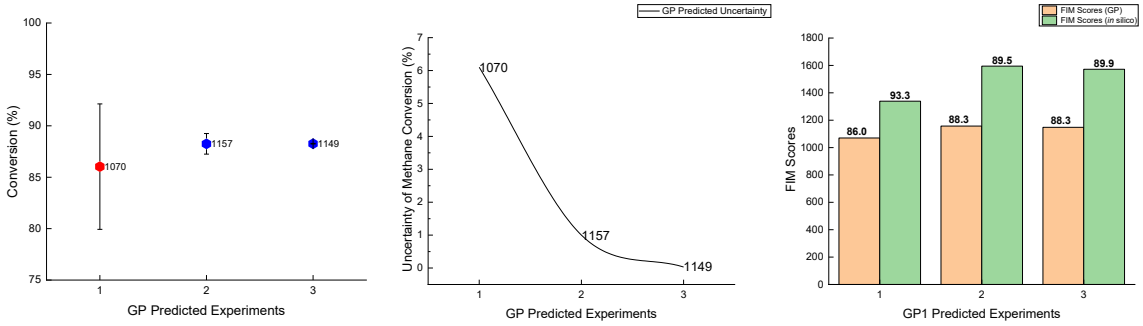
3.1 Performance of GP1

Using the GP1–GP2 workflow, GP1 was used to design three optimal experiments in sequence. For Experiments 1–3, the predicted conversions were 86.0%, 88.3%, and 88.3%. The inversion of GP1 provided estimated FIM scores of 1070, 1157, and 1148, respectively showing that each experiment was not only high in conversion but also valuable for improving the model by providing more information. While Experiments 1 and 2 exceeded the 1% uncertainty threshold (±18.40% and ±2.27%), Experiment 3 met the stopping criterion (±0.03%) – which was well below the 1% threshold. The reactor conditions estimated from GP2 inversion, presented in Table 2, showed consistent convergence within the design space, this suggests that the model consistently identified region with optimal and informative condition. Figure 2a shows how GP1 captures a clear trend between FIM scores and predicted methane conversion, as FIM score increases, so also conversion, particularly in the 1000-1200 FIM range where conversions exceed 86%. Corresponding predictive uncertainties show a sharp decline with increasing FIM values from ±18.40% to ±0.03% as seen in 86.0 ± 18.40, 88.3 ± 2.27, and 88.3 ± 0.03. The sharp uncertainty reduction (from ±18.40% to ±0.03%) occurs because the optimized GP1 preferentially sampled high-conversion regions where the Fisher information content was the highest, leading to progressively more confident predictions after each iteration. Figure 2b further describes the GP model's

tendency to yield lower uncertainty near informative, well-sampled regions. While promising, this correlation should be further validated in more complex reaction systems to confirm its general applicability.

3.2 GP1 Validation with In-silico Experiments

The predictions from GP1 were validated using in silico experiments, confirming alignment between model outputs and simulated results. Figure 2c illustrates how the predicted methane conversions and FIM scores from GP1 closely matched the corresponding in silico values. For Experiments 1, 2, and 3, GP1 estimated FIM scores of 1070, 1157, and 1149, while the in-silico values were 1339, 1595, and 1572, respectively. A similar trend was observed in conversion outcomes, supporting the reliability of the model, the predicted conversions were 86.0%, 88.3%, and 88.3%, compared to in silico conversions of 93.3%, 89.5%, and 89.9%. This consistency supports the reliability of the integrated GP1–GP2 modelling framework in guiding experimental optimization, even across different prediction and validation stages.



(a) *(b)* *(c)*

Figure 2: (a) GP-predicted conversions for Experiments 1-3 (colour bar: absolute FIM scores). (b) Corresponding predicted uncertainties, showing inverse relationship with FIM scores (as reported). (c) Comparison of FIM scores predicted by GP1 and validated through in silico experiments for experiments 1–3. The bar chart shows GP1-predicted FIM scores (orange) alongside their corresponding in silico values (green).

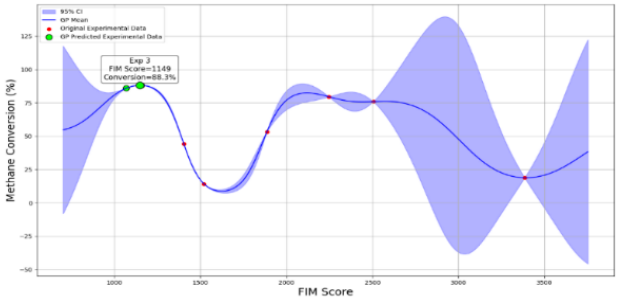


Figure 3. GP1 model predictions after Iteration 3 showing methane conversion as a function of FIM score. The model's predicted 95% confidence interval (shaded region) narrows as uncertainty decreases.

Table 2: Predicted Reactor Conditions using Integrated Workflow of GP1 & GP2. Conversion in percentage (%)

Pred Exp	Temp ℃	Mass flow (mL/min)	O_2/CH_4 Ratio (mol/mol)	Inlet CH_4 Concentration (mol/mol)	FIM scores (GP)	FIM scores (in silico)	GP predicted Methane Conversion	In-silico Methane Conversion
1	347.9	20.6	2.19	0.023	1070	1339	86.0±18.40	93.3
2	345.0	20.73	2.18	0.023	1157	1595	88.3± 2.27	89.5
3	345.3	20.72	2.18	0.023	1148	1572	88.3± 0.03	89.9

3.3 GP1 Optimal Experiment Design & Procedure Termination

The third iteration (Experiment 3) of the optimized GP1 yielded a predicted methane conversion of 88.3%, paired with a high FIM score of 1148.8 and a very low uncertainty of 0.03%. This met the stopping criterion, as the uncertainty fell below the 1% threshold, prompting termination of the optimization process. Additionally, Figure 3 illustrates that the confidence interval was significantly reduced, closely aligning with the GP mean line, which further confirms the reliability of the prediction.

3.4 Performance of GP2

Prior to establishing the GP1–GP2 workflow, GP2 was validated by estimating the FIM for a new reactor condition: 277°C, 24.4 mL/min, a 3.4 mole ratio, and a 0.024 inlet CH_4 concentration. The true FIM, obtained from in silico experiments, was 307, compared to GP2's prediction of 294 ± 9.0. This close agreement supports GP2's reliability in guiding experimental design.

4. Conclusion

A hybrid modelling workflow leveraging Gaussian Process (GP) regression and optimal experimental design has been proposed in this paper and applied to the optimization of a reactor for the catalytic oxidation of methane in flow. The approach was used to design a sequence of three experiments starting from a preliminary set of thirty baseline experiments. Results show that experiments selected based on higher FIM scores consistently led to improved methane conversion, validating the use of FIM as optimal design criterion. GP Predicted Experiment 1 achieved a conversion of 86.0% ± 18.40% (GP prediction) versus 93.3% (in silico experiment), with a FIM score of 1070 and 1339 respectively showing close match between GP predictions, and in silico outcomes. A clear trend emerged across all experiments: as FIM score increased, methane conversion also improved. This correlation confirms that information-rich conditions not only enhance parameter identifiability but also drive reactor performance toward optimal regimes. The highest observed FIM corresponded to a near-optimal conversion of 89.5%, underscoring the effectiveness of the GP-informed experimental design. These findings position the FIM score as a potential metric for guiding data-driven optimization in catalytic reaction systems. However, the current study is limited by the relatively small size of the experimental dataset, which may affect the generalizability and robustness of the GP models. Future work will focus on i) extending this workflow to more complex systems, including dynamic or multi-step reactions; ii) exploring multi-objective design scenarios; iii) expanding the experimental dataset to improve model generalizability; iv) benchmarking the proposed approach against other uncertainty quantification methods such as Bayesian neural networks and Markov Chain Monte Carlo.

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