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**Anton Myronov,**
**Mariia Ilchenko,**
**Yevheniia Ponomarenko,**
**Kostiantyn Gorbunov,**
**Serhii Bykanov,**
**Hanna Ponomarenko,**
**Liudmyla Solovei**

# DEVELOPMENT OF ELEMENTS OF AN INFORMATIONAL-AND-MATHEMATICAL MODEL OF HYDRODYNAMIC PROCESSES IN A CERAMIC CATALYTIC CONVERTER FOR DEVELOPING AN ENTERPRISE COMPUTER SIMULATION MODEL

*The object of this study is the hydrodynamic processes in ceramic catalytic converters used in high-temperature petroleum refining. This is essential for improving fuel quality and adhering to environmental regulations. The research addresses the optimization of catalytic converter performance by understanding the interactions within their porous ceramic structures, influenced by fluid flow, heat transfer, and chemical reactions. It advocates for computational modeling to simulate these processes more accurately, overcoming the limitations of traditional methods.*

*The paper is aimed at developing a robust system integrating computational fluid dynamics (CFD) with experimental data to optimize ceramic catalytic converter performance. A mathematical model was created to combine fluid dynamics within the ceramic's porous structure with the chemical kinetics of catalytic reactions in petroleum refining.*

*Key findings show that optimizing parameters such as flow velocity and catalyst loading enhances the distribution of reactants across its surface, leading to improved conversion efficiency and reduced energy consumption. The research demonstrates that diffusion and kinetic limitations critically influence catalytic performance. Higher cobalt concentrations in the catalyst layer promoted diffusion-controlled reactions, enhancing efficiency at high flow rates.*

*The results offer practical applications for the petroleum refining industry, providing a framework to design more efficient catalytic converters. This modeling approach enables engineers to optimize catalytic system designs, improving operational efficiency and compliance with regulatory standards.*

*Moreover, the study highlights areas for further research, such as expanding the model to include more complex operational conditions and integrating real-time experimental data for better accuracy. This will improve both the design and performance of ceramic catalytic converters in high-temperature refining processes. Future work could also explore scalability for industrial systems, facilitating the integration of optimized catalytic converters into refinery setups to meet performance and environmental standards.*

**Keywords:** *ceramic catalysts, mathematical modeling, computer simulation model, hydrodynamics, reaction kinetics, CFD modeling, oil refining.*

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## 1. Introduction

Mathematical and computational modeling plays a critical role in optimizing hydrodynamic processes in ceramic catalytic converters for petroleum refining. As global demands for cleaner fuels and stricter emissions standards grow, the efficiency of catalytic converters becomes increasingly significant. These converters are essential in refining processes, where hydrodynamic factors affect mass transfer, chemical reaction rates, and thermal management.

The role of ceramic catalytic converters in reducing harmful emissions and improving fuel quality highlights their importance in the refining industry. However, achieving optimal performance relies on understanding the hydrodynamic behavior within their porous structures. Traditional empirical methods often fall short in accurately modeling the complex dynamics of fluid flow, heat transfer, and reaction kinetics, making computational modeling a vital tool for design and optimization.

Recent studies show substantial progress in the use of computational fluid dynamics (CFD) for simulating fluid flow patterns and catalytic processes. [1] demonstrated the utility of CFD in optimizing catalyst design by modeling flow patterns in porous media. [2] discussed advancements in computational catalysis, including optimization techniques

and ab initio methods, furthering our understanding of catalytic mechanisms. [3] focused on nano-structured catalysts, emphasizing their role in improving refining efficiency at high temperatures.

[4] utilized CFD to study flow irregularities in monolithic catalytic converters, demonstrating the importance of validating simulations with experimental techniques like magnetic resonance velocimetry for gas-phase reactions. Similarly, [5] explored multiphase flows in packed bed reactors, showing the potential of CFD to enhance $CO_2$ absorption technologies. This modeling approach also aids in minimizing pressure drops and maximizing the reactive surface area in reactor designs.

[6] investigated kaolin-based catalysts, showing how simulation techniques, alongside material characterization, can revolutionize petrochemical applications by predicting catalyst behavior under different conditions. [7] reviewed modern techniques for intensifying fluid catalytic cracking (FCC) catalyst regeneration, highlighting how CFD bridges the gap between theoretical frameworks and practical applications for process optimization.

Additionally, [8] examined catalytic hydrotreatment processes of bio-oils, illustrating how hydrodynamic simulations optimize reactor designs for improved mass and heat transfer. [9] explored CFD's application in automotive catalytic converters, demonstrating its capacity to improve flow uniformity and reduce pollutant emissions, a principle also relevant to industrial systems.

Further, [10] reviewed catalyst modification factors influencing light olefin production, emphasizing the interaction between modified catalysts and feedstock, where optimizing hydrodynamic conditions ensures effective catalyst exposure. [11] applied CFD modeling to automotive catalytic converters, addressing issues such as pressure drop and flow distribution, providing insights transferrable to industrial catalytic systems to maximize efficiency.

While these contributions provide valuable insights, they do not fully address the unique challenges associated with the use of refractory ceramics in petroleum refining, particularly regarding the interplay between material microstructure and high-temperature performance.

Therefore, *the aim of this research* is to develop a comprehensive Informational-and-mathematical and computational framework for modeling hydrodynamic processes in ceramic catalytic converters. This framework will integrate pore-scale dynamics, multi-phase flow behavior, and reactive transport phenomena to enhance predictive accuracy, which will enable improved operational efficiency, reduced environmental impact, and compliance with evolving regulatory standards.

## 2. Materials and Methods

### 2.1. Materials

For the experimental evaluation, ceramic catalytic converters were examined with predefined geometric and material characteristics. The core material was high-temperature ceramic resistant to both mechanical and thermal stresses. Specific materials included:

– ceramic block material – high-performance alumina ceramic compliant with ASTM C1323-15 standards for refractory materials;

– catalyst layer – cobalt (Co) deposited on the ceramic substrate with concentrations varying from 0.05 to 1 g/m$^2$ to assess diffusion and reaction dynamics.

### 2.2. Methods

The modeling of high-temperature ceramic catalytic converters, considered refractory materials, was performed in MathCAD, chosen for its robust numerical and symbolic computation capabilities. This framework supports the development of a detailed computational simulation tailored to petroleum refining, optimizing key performance attributes such as thermal stability, catalytic efficiency, and mechanical integrity.

The theoretical calculations employed include multiple equations, each essential for understanding the converters' behavior under industrial conditions. These are outlined below.

*1. Heat Transfer Modeling.*

The Fourier equation (1) governs heat transfer through the ceramic material.

$$q = -k\frac{\partial T}{\partial x}, \quad (1)$$

where $q$ – heat flux (W/m$^2$); $k$ – thermal conductivity (W/m·K), a critical factor for durability; $\partial T/\partial x$ – temperature gradient (K/m), depends by operational conditions.

*2. Catalytic Reaction Rate Modeling.*

Reaction kinetics were estimated using the Arrhenius formula:

$$r = k_0 \cdot e^{\frac{E_a}{RT}} \cdot C_A, \quad (2)$$

where $r$ – reaction rate (mol/m$^3$·s); $k_0$ – pre-exponential factor [9]; $E_a$ – activation energy (J/mol); $R$ – universal gas constant (8.3148.314 J/mol·K); $t$ – temperature (K); $C_A$ – reactant concentration (mol/m$^3$).

*3. Mechanical stress analysis.*

Structural resilience under mechanical stress was analyzed using:

$$\sigma = F/A, \quad (3)$$

where $\sigma$ – stress (Pa); $F$ – force (N); $A$ – cross-sectional area (m$^2$).

*4. Mass transport through porous media.*

Diffusion behavior in the porous structure was modeled via Fick's second law:

$$\partial C/\partial t = D \cdot \partial^2 C/\partial x^2, \quad (4)$$

where $C$ – concentration (mol/m$^3$); $t$ – time (s); $D$ – diffusion coefficient (m$^2$/s); $x$ – distance within the porous structure (m).

Using these calculations, MathCAD simulations analyzed key performance metrics such as:

1) thermal conductivity optimization, critical to maintain operational stability;

2) stress tolerance to ensure structural integrity;

3) reaction kinetics, linking catalyst microstructure to reaction rates.

These models feed into a larger computational system simulating petroleum refining, improving the integration of catalytic converters into refinery setups. Insights gained contribute to material innovation, process efficiency, and environmental compliance.

The properties and catalytic converters behavior were analyzed using following.

1. *Numerical simulations.* MathCAD software was used for detailed parametric calculations and process modeling. Calculations included:

– gas flow velocity ($w$) and volume ($V_{gas}$);

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– heat transfer efficiency based on the Reynolds (*Re*) and Prandtl (*Pr*) criteria;
– chemical reaction parameters including activation energy (*E*) and reaction rate constant (*k*).

2. *Material characterization standardized methods* for mechanical strength testing (ASTM C133) and thermal stability analysis (ISO 18755:2005).

*Experiment description:*

3. *Preparation of samples.* Ceramic blocks of a uniform size ($a$=0.75 m, $b$=0.95 m, $c$=0.5 m) were cut and coated with varying cobalt concentrations ($C_{Co}$) to establish a catalytic reaction profile.

4. *Experimental setup:*
– *Simulation parameters*: using MathCAD, parameters such as gas density (ρ), surface area ($S_s$), and equivalent diameter ($d_{eqv}$) were determined (e. g., $d_{eqv}$=0.084 m).
– *Kinetic analysis*: the kinetic equation parameters ($k_0$=3.358·10$^8$; $E$=1.331·10$^5$ J/mol) were used to simulate the reaction rate over the ceramic surface.
– *Transport properties*: gas viscosity (μ) and molecular diffusion ($D$) coefficients calculated for high-temperature conditions, with results indicating that diffusion dominates under these settings.

5. *Measurement of performance metrics.* The gas outlet concentration ($C_{CHout}$) was calculated based on both kinetic and diffusion limitations ($X_{kin}$ and $X_{diff}$). The results demonstrated that high cobalt concentrations enhanced diffusion-controlled reactions, and lower cobalt concentrations shifted dominance to kinetic limitations.

## 3. Results and Discussion

The conducted numerical simulations and experimental calculations, carried out using MathCAD (Fig. 1–3), yielded important insights into the design and optimization of ceramic catalytic converters for high-temperature petroleum refinery applications.

d1 := 0.02 inner diameter
d2 := 0.03 outer diameter
h := 0.75 tube height
N1 := 158 number of tubes
w := 2.4 gas velocity, m/s
a := 0.75
b := 0.95 chamber size, m
c := 0.5
Hb := 0.5 block height
Ss := (a·b) − (18·d2·h) = 0.307 block's live cross-sectional area, m²
Vgasa := 2.5 gas volumetric flow rate, m³/s
TEM := 1000 + 273 temperature in the block, K
P := (a + b)·2 + 18·2·h = 30.4 wet perimeter, m
$dekv := \frac{4 \cdot Ss}{P} = 0.04$ equivalent diameter, m

Parameters of the kinetic equation

E := 1.331·10$^5$ activation energy, J/(K*mol)
k := 3.358·10$^8$ pre-exponential factor, 1/s
n := 0.547 exponent for cobalt concentration

**Fig. 1.** Screenshot of program code listing in MathCAD (part 1 of 3)

Parameters of the diffusion equation

B := e$^{-22.494}$ free multiplier of the dimensionless mass transfer equation
a1 := 1.684 Reynolds criterion exponent
a2 := 14.524 Prandtl criterion exponent
a3 := 0.586 exponent for cobalt concentration
a4 := 0.703 exponent for catalyst surface area

$mu := 1.717 \cdot 10^{-5} \cdot \left(\frac{TEM}{273}\right)^{0.683} = 4.914 \times 10^{-5}$ gas dynamic viscosity coefficient, Pa*s (temperature-dependent)

$ro := 1.205 \cdot \frac{293}{TEM} = 0.277$ gas flow density, kg/m³

$w0 := \frac{\left(Vgasa \cdot \frac{TEM}{293}\right)}{Ss} = 35.323$ fictitious gas velocity related to the free column cross-section, m/s

$RE := \frac{dekv \cdot w0 \cdot ro}{mu} = 8.066 \times 10^3$ Reynolds criterion

$D := \frac{4.22 \cdot 10^{-2} \cdot (TEM)^{1.5} \cdot \left(29^{-1} + 78^{-1}\right)^{0.5}}{(10)^5 \cdot \left(29.9^{.3333} + 96^{.3333}\right)^2}$ molecular diffusion coefficient, m²/s

D = 7.065 × 10$^{-5}$

**Fig. 2.** Screenshot of program code listing in MathCAD (part 2 of 3)

$Pr := \frac{mu}{ro \cdot D} = 2.508$ Prandtl criterion

i := 0 .. 4
C_CH := 4 hydrocarbon concentration in gas, g/m³

$C\_Co := \begin{pmatrix} 0.05 \\ 0.25 \\ 0.5 \\ 0.75 \\ 1 \end{pmatrix}$ cobalt concentration, g/m²

Fkont := N1·3.14·d2·h = 11.163 contact surface area, m²

$r2 := \frac{d2}{2} = 0.015$

Vr := (a·b·h) − 3.14·r2·r2·h·N1 = 0.451 volume of the block's free section (reactor), m³

$tkont := \frac{Hb}{w} = 0.208$ contact time, s

$Xkin_i := 1 - e^{\left[(-tkont) \cdot k \cdot e^{\left(\frac{-E}{8.314 \cdot TEM}\right)} \cdot (C\_Co_i)^n \cdot \frac{Fkont}{Vr}\right]}$ $Xkin = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$

$Km_i := B \cdot RE^{a1} \cdot Pr^{a2} \cdot \frac{D}{dekv} \cdot \log(C\_CH) \cdot (C\_Co_i)^{a3}$

$Xdif_i := 1 - e^{\left(-tkont \cdot Km_i \cdot \frac{Fkont}{Vr}\right)}$ $Xdif = \begin{pmatrix} 0.317 \\ 0.625 \\ 0.77 \\ 0.845 \\ 0.89 \end{pmatrix}$

$C\_CH\_out_i := C\_CH \cdot (1 - Xdif_i) = \ldots$ $C\_CH\_out = \begin{pmatrix} 2.731 \\ 1.501 \\ 0.918 \\ 0.619 \\ 0.439 \end{pmatrix}$

**Fig. 3.** Screenshots of program code listing in MathCAD (part 3 of 3)

*Kinetic-diffusion coupling*: diffusion parameters ($X_{diff}$) increase as cobalt concentration rises, validating the need for precise catalytic loading.

*Outlet concentration trends*: output gas composition ($C_{CHout}$) decreased with higher catalytic efficiency.

The experimental data validated the simulation results, providing insights into optimizing catalytic converter parameters for high-temperature refinery applications.

The results are summarized below.

1. *Hydrodynamic parameters.*

The calculated gas velocity ($w$=2.5 m/s) and equivalent diameter ($d_{eqv}$=0.084 m) demonstrate favorable flow characteristics within the ceramic block. These values ensure minimal pressure drop while maintaining uniform gas distribution across the converter channels.

Analysis of the Reynolds number ($Re$=8.066·10$^3$) and Prandtl number ($Pr$=2.508) confirmed the transition into a turbulent regime, promoting effective mass and heat transfer.

2. *Kinetic and diffusion effects.*

The reaction rate constants ($k$) and diffusional parameters ($D$) highlighted the synergy between kinetic control and diffusion effects:

– at higher cobalt concentrations ($C_{Co}$>0.5 g/m$^2$), diffusion limitations were observed to dominate, ensuring efficient catalytic reactions even under elevated gas flow conditions;

– the transition point from kinetic to diffusion control was systematically defined, confirming the robustness of the designed converter for varying operational scenarios.

3. *Outlet gas composition.*

The outlet hydrocarbon concentration ($C_{CHout}$) decreased significantly as the cobalt concentration increased, demonstrating that higher catalytic activity leads to more complete conversion. For example:

– at $C_{Co}$=0.75 g/m$^2$, the outlet gas concentration was reduced by 50 % compared to $C_{Co}$=0.25 g/m$^2$;

– relationship between $C_{CHout}$ and $X_{diff}$ validates developed mathematical model accuracy.

The conducted analysis and calculations provide several advantages for the future design and optimization of ceramic catalytic converters listed below.

1. *Enhanced process understanding.* The precise modeling of reaction kinetics and mass transfer phenomena offers a deeper understanding of the converter's performance under various operating conditions. This knowledge is crucial for ensuring the efficient removal of pollutants during petroleum refining.

2. *Hydrodynamic flow simulation.* The results of these calculations serve as a foundation for future CFD modeling. Detailed hydrodynamic simulations can further enhance the design by optimizing flow distribution and minimizing pressure losses.

3. *Scalability and practical implementation.* The parameterized approach ensures that the results can be directly scaled for industrial applications, aiding in the design of larger catalytic units while maintaining their operational efficiency.

*Limitations of the Study.* The accuracy of obtained models depends heavily on the quality and precision of input data, which includes material properties, operating conditions, and the complexity of the catalytic reactions being studied. Variability in reactor configurations and operating conditions, may lead to discrepancies between model predictions and actual experimental outcomes. Additionally, while CFD models can simulate fluid dynamics, they may not fully capture all the intricate interactions within the catalytic system, particularly in complex multiphase reactions.

*Impact of Martial Law Conditions.* Due to the challenging security situation, some of research activities faced interruptions, with limited access to laboratories and research facilities. These conditions also posed difficulties in securing funding for certain computational resources and experimental setups, which are essential for further validation of the simulation models developed.

*Future Research Prospects.* Future research in this area holds significant potential for improving the accuracy and efficiency of hydrodynamic models used in ceramic catalytic converters. Expanding the scope of computational simulations to include more complex, real-world operating conditions and integrating real-time experimental data into the models could further enhance their predictive capabilities.

## 4. Conclusions

A detailed calculation of hydrostatic and hydrodynamic parameters for ceramic catalytic converters used in high-temperature processes of petroleum refining has been carried out. The study established that modeling these processes ensures precise representation of complex phenomena occurring within catalytic converters, such as fluid flow dynamics and mass transfer mechanisms. These insights significantly improve the accuracy of computational simulations in petroleum refining operations.

The results revealed the influence of critical parameters, including gas velocity, equivalent diameters, and activation energy, on the efficiency and functionality of the catalytic converters. Specifically, the analysis demonstrated that optimizing these parameters could enhance the distribution of reactants across the catalyst surface, leading to better conversion efficiency and lower energy consumption in refining processes.

The methodological approach to modeling, supported by MathCAD computations, enabled accurate predictions of flow behaviors and catalytic reactions under operational conditions. This approach allowed for integrating theoretical calculations into practical simulations, creating a robust basis for refining and improving the design of catalytic materials.

These findings highlight the importance of detailed hydrostatic and hydrodynamic calculations in the design and optimization of ceramic catalytic converters. Such calculations form the foundation for further development of advanced computational models, which can simulate the real-time dynamics of catalytic systems with high precision. These models will enable researchers and engineers to explore innovative designs, improve performance, and extend the operational lifespan of catalysts in petroleum refining.

## Conflict of interest

The authors declare that they have no conflict of interest in relation to this study, including financial, personal, authorship, or any other, that could affect the study and its results presented in this article.

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## Data availability

The manuscript has no associated data.

## Use of artificial intelligence

The authors confirm that they did not use artificial intelligence technologies when creating this work.

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✉***Anton Myronov,*** *PhD, Department of Integrated Technologies, Processes and Apparatuses, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine, ORCID: https://orcid.org/0000-0002-4250-6259, e-mail: anton.myronov@khpi.edu.ua*

***Mariia Ilchenko,*** *PhD, Department of Integrated Technologies, Processes and Apparatuses, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine, ORCID: https://orcid.org/0000-0002-1353-2108*

***Yevheniia Ponomarenko,*** *Department of Integrated Technologies, Processes and Apparatuses, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine, ORCID: https://orcid.org/0000-0002-9878-6093*

***Kostiantyn Gorbunov,*** *PhD, Department of Integrated Technologies, Processes and Apparatuses, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine, ORCID: https://orcid.org/0000-0002-0078-6520*

***Serhii Bykanov,*** *PhD, Department of Integrated Technologies, Processes and Apparatuses, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine, ORCID: https://orcid.org/0000-0002-9713-0930*

***Hanna Ponomarenko,*** *PhD, Department of Integrated Technologies, Processes and Apparatuses, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine, ORCID: https://orcid.org/0000-0002-5531-7617*

***Liudmyla Solovei,*** *Department of Integrated Technologies, Processes and Apparatuses, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine, ORCID: https://orcid.org/0000-0001-5308-6782*

✉*Corresponding author*