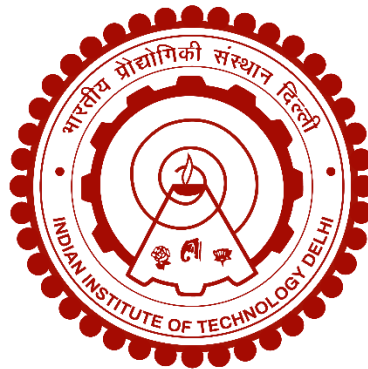


**HYDRODYNAMICS OF THREE PHASE RADIAL
FLOW REACTOR: EXPERIMENTS AND REACTOR
MODEL FOR HYDROPROCESSING**

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**DEPARTMENT OF CHEMICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY DELHI**

MARCH 2023

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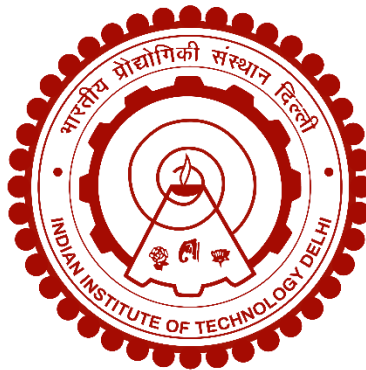
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Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy

to the



Indian Institute of Technology Delhi

March 2023

Dedicated to my Wife, Pranjal

for her endless love, support, and encouragement.

CERTIFICATE

This is to certify that the thesis entitled “**Hydrodynamics of Three Phase Radial Flow Reactor: Experiments and Reactor Model for Hydroprocessing**”, being submitted by **Prashant Udaysinh Parihar** to the Indian Institute of Technology Delhi, is worthy of consideration for the award of the degree of **Doctor of Philosophy** and is a record of the original bonafide research work carried out by him under our guidance and supervision. The results contained in the thesis have not been submitted in part or full, to any other University or Institute for the award of any degree or diploma. We certify that he has pursued the prescribed course of research.

Date: 15th March 2023



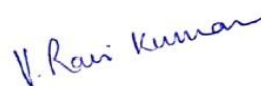
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Thanks again for all the support and encouragement.

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Prashant Udaysinh Parihar

ABSTRACT

Trickle bed reactors (TBR) are widely used in refining industry for hydroprocessing (desulphurization, denitrogenation, olefin saturation, dearomatization, hydrocracking, and isomerization) of hydrocarbon feedstock to meet requirements of cleaner fuels and production of high-quality base oils for lubricants. TBR is operated in an adiabatic mode with intermediate quenching to check the rise in temperature due to the exothermic hydrogenation reactions. Trickle bed reactors are limited by excess hydrogen (Gas/Oil ratio: 400 to 1200 Nm³/m³), high bed pressure drop, large recycle of unreacted hydrogen, feed vaporization, reducing hydrogen partial pressure and increasing hydrogen partial pressure along height, etc. This is often compensated by large reactors (higher catalyst requirement) and high severity operation to meet product quality specifications which in turn leads to non-selective cracking of hydrocarbon feedstock to light ends and shorter run lengths.

To overcome these limitations of TBR, the three-phase radial flow reactor (RFR) is conceptualized in the literature. Although two-phase (gas-solid) radial flow reactors are commercially used for applications such as naphtha reforming process and ammonia synthesis, gas-liquid-solid radial flow reactor is unexplored field till date. RFR is a packed bed reactor with an annular bed of catalyst, liquid feed trickles downward while gas is introduced through a central gas distributor extending vertically downward. Gas flows in radially outward direction across catalyst bed. RFR configuration results in lower pressure drop due to reduced flow path, higher partial pressure of hydrogen along height, simultaneous reaction, and separation of gas phase products such as H₂S and NH₃ and minimization of inhibition effects. In spite of these features, experimental and modeling studies for RFR are lacking in comparison to TBR. Therefore, it is

important to validate and understand RFR configuration through experimental and simulation studies.

In the present work experimental investigations of gas-liquid flow were carried out in laboratory scale radial flow and trickle bed reactor packed with commercial hydroprocessing catalyst. Experimentally identified critical limitation of radial flow reactor in terms of allowable liquid and gas flow rate (operating range) without causing radial displacement of liquid out of the bed (termed as weeping; undesired operation). Effects of reactor internals, bed porosity, flow arrangements and gas-liquid flow rates were investigated on operating range. Measurements of pressure drop, liquid hold-up, residence time distribution and axial dispersion were carried out with variation in gas and liquid flow rates. Analyzed sensitivity of weeping to gas and liquid flow rates till maximum possible liquid displacement from RFR. Based on experimental data, empirical correlations were proposed for predicting liquid hold-up and two-phase pressure drop. Further, experimental investigations were performed to assess pressure drop, liquid hold-up, residence time distribution and axial dispersion of RFR vis a vis TBR. These studies form the database critical for design and performance evaluation of novel radial flow configuration.

Another focus of the thesis was to develop 1-D and 2-D reactor model for predicting performance of commercial scale RFR for diesel hydroprocessing. To achieve this objective, first 1-D model for commercial scale TBR was developed and validated using literature reported kinetic data. To separate intrinsic kinetics from apparent kinetics in data, wetting efficiency and effectiveness factor were incorporated in the model. Literature reported mixing cell network consisting of string of CSTR's has been adopted for the model development. Post validation of 1-D reactor model of TBR, 1-D reactor model developed for RFR using intrinsic kinetic data. Simulation studies were performed for RFR and compared its performance with TBR. 1-D models

predicted profiles for concentration of reacting species, temperature, partial pressure of H₂ and H₂S and effectiveness factor along reactor height. Further, to assess impact of maldistribution of liquid which is relevant in the real world; 1-D models were extended to 2-D geometry for TBR and RFR. The 2-D model simulated impact of change in liquid and gas distribution at the reactor inlet on the species concentration and temperature profile along reactor height and diameter. Maldistribution factor Mf was varied in the range 0-0.6 to analyze effect of maldistribution in liquid phase on performance of TBR and RFR in terms sulfur content (ppm) in outlet stream from the reactor. Further, 2-D model developed for TBR in the present study can be used to determine extent of maldistribution and probable size of hot zone based on measured axial and radial temperature profile in the commercial scale TBR. 2-D model of RFR can be used to assess safe and feasible operation with allowed degree or limit for liquid maldistribution.

The unique aspect of this thesis lies in the fact that it is the principal research study focusing on experimental and simulation studies for the three-phase radial flow reactor for hydroprocessing.

सार

ट्रिकल बेड रिएक्टरों (टीबीआर) का व्यापक रूप से हाइड्रोप्रोसेसिंग (डीसल्फराइजेशन, डिनिटोजेनाइजेशन, ओलफिन सैचुरेशन, डिओरेमेटाइजेशन, हाइड्रोक्रैकिंग और आइसोमराइजेशन) हाइड्रोकार्बन फीडस्टॉक के लिए रिफाइनिंग उद्योग में व्यापक रूप से उपयोग किया जाता है ताकि क्लीनर ईंधन की आवश्यकताओं को पूरा किया जा सके और लुब्रिकेंट के लिए उच्च गुणवत्ता वाले आधार तेलों का उत्पादन किया जा सके। टीबीआर में, गैस और तरल गैस-तरल वितरक के माध्यम से ऊपर से रिएक्टर में प्रवेश करते हैं, उत्प्रेरक बिस्तर के माध्यम से कोकरेंट डाउन फ्लो मोड में बहते हैं। टीबीआर को एकसोथर्मिक हाइड्रोजनीकरण प्रतिक्रियाओं के कारण तापमान में वृद्धि की जांच करने के लिए मध्यवर्ती शमन के साथ एक आदिबाटिक मोड में संचालित किया जाता है। मिलने वाले बिस्तर रिएक्टर अतिरिक्त हाइड्रोजन (गैस/तेल अनुपात: 400 से 1200 एनएम³/एम³), उच्च बिस्तर दबाव ड्रॉप, अप्रतिरक्षित हाइड्रोजन का बड़ा रीसायकल, फीड वाष्पीकरण, हाइड्रोजन आंशिक दबाव को कम करने और ऊंचाई के साथ हाइड्रोजन आंशिक दबाव बढ़ाने आदि द्वारा सीमित हैं। यह अक्सर बड़े रिएक्टरों (उच्च उत्प्रेरक आवश्यकता) और उत्पाद की गुणवत्ता विनिर्देशों को पूरा करने के लिए उच्च गंभीरता आपरेशन द्वारा मुआवजा दिया जाता है।

टीबीआर की इन सीमाओं को दूर करने के लिए साहित्य में तीन चरण रेडियल फ्लो रिएक्टर (आरएफआर) की संकल्पना की जाती है। यद्यपि दो चरण (गैस-ठोस) रेडियल फ्लो रिएक्टरों का

व्यावसायिक रूप से नेफ्था सुधार प्रक्रिया और अमोनिया संश्लेषण जैसे अनुप्रयोगों के लिए उपयोग किया जाता है, गैस-तरल-ठोस रेडियल प्रवाह रिएक्टर आज तक बेरोज़गार क्षेत्र है । आरएफआर उत्प्रेरक के एक वलयाकार बिस्तर के साथ एक पैक बिस्तर रिएक्टर है, तरल फ़ीड नीचे की ओर जाता है जबकि गैस को एक केंद्रीय गैस वितरक के माध्यम से पेश किया जाता है जो लंबवत नीचे की ओर बढ़ा है। गैस उत्प्रेरक बिस्तर के पार मूल रूप से जावक दिशा में बहती है । आरएफआर विन्यास के परिणामस्वरूप कम प्रवाह पथ, ऊंचाई के साथ हाइड्रोजन का उच्च आंशिक दबाव, एक साथ प्रतिक्रिया और एच₂एस और एनएच₃ जैसे गैस चरण उत्पादों को अलग करने और अवरोध प्रभावों को कम करने के कारण कम दबाव में गिरावट आती है । इन फीचर्स के बावजूद टीबीआर की तुलना में आरएफआर के लिए एक्सपेरिमेंटल और मॉडलिंग की पढ़ाई में कमी है। इसलिए प्रयोग के माध्यम से आरएफआर विन्यास को मान्य और समझना महत्वपूर्ण है।

वर्तमान कार्य में गैस-तरल प्रवाह की प्रायोगिक जांच प्रयोगशाला स्केल रेडियल फ्लो और ट्रिकल बेड रिएक्टर में वाणिज्यिक हाइड्रोप्रोसेसिंग उत्प्रेरक के साथ पैक की गई थी। बिस्तर से तरल के रेडियल विस्थापन के बिना स्वीकार्य तरल और गैस प्रवाह दर (ऑपरेटिंग रेंज) के संदर्भ में रेडियल फ्लो रिएक्टर की प्रायोगिक रूप से महत्वपूर्ण सीमा की पहचान की गई (जिसे रोना; अवांछित ऑपरेशन कहा जाता है)। ऑपरेटिंग रेंज पर रिएक्टर इंटरनल, बेड सरंधता, प्रवाह व्यवस्था और गैस-तरल प्रवाह दरों के प्रभावों की जांच की गई। गैस और तरल प्रवाह दरों में भिन्नता के

साथ दबाव ड्रॉप, तरल होल्डअप, निवास समय वितरण और अक्षीय फैलाव का मापन किया गया। RFR से अधिकतम संभव तरल विस्थापन तक गैस और तरल प्रवाह दर के प्रति रोलने की संवेदनशीलता का विश्लेषण किया। प्रायोगिक आंकड़ों के आधार पर, तरल होल्ड अप और दो चरण दबाव ड्रॉप की भविष्यवाणी के लिए अनुभवजन्य सहसंबंध प्रस्तावित किए गए थे। इसके अलावा, दबाव ड्रॉप, लिक्विड होल्ड अप, निवास समय वितरण और टीबीआर की तुलना में आरएफआर के अक्षीय फैलाव का आकलन करने के लिए प्रायोगिक जांच की गई। ये अध्ययन उपन्यास रेडियल प्रवाह विन्यास के डिजाइन और प्रदर्शन मूल्यांकन के लिए महत्वपूर्ण डेटाबेस बनाते हैं।

शोध प्रबंध का एक अन्य लक्ष डीजल हाइड्रोप्रोसेसिंग के लिए वाणिज्यिक पैमाने के आरएफआर के प्रदर्शन की भविष्यवाणी के लिए 1-डी और 2-डी रिएक्टर मॉडल विकसित करना था। इस उद्देश्य को प्राप्त करने के लिए, व्यावसायिक पैमाने के टीबीआर के लिए पहला 1-डी मॉडल विकसित किया गया था और साहित्य रिपोर्ट किए गए गतिज डेटा का उपयोग करके मान्य किया गया था। डेटा में स्पष्ट कैनेटीक्स से आंतरिक कैनेटीक्स को अलग करने के लिए, मॉडल में गीला दक्षता और प्रभावशीलता कारक शामिल किया गया था। लिटरेचर रिपोर्टेड मिक्सिंग सेल नेटवर्क जिसमें CSTR की स्ट्रिंग शामिल है, को मॉडल विकास के लिए अपनाया गया है। टीबीआर के 1-डी रिएक्टर मॉडल के स्थापन के बाद, आंतरिक गतिज डेटा का उपयोग करके आरएफआर के लिए विकसित 1-डी रिएक्टर मॉडल। आरएफआर के लिए सिमुलेशन अध्ययन किया गया और

टीबीआर के साथ इसके प्रदर्शन की तुलना की गई। 1-डी मॉडल ने प्रतिक्रियाशील प्रजातियों की सांद्रता, तापमान, एच₂ और एच₂एस के आंशिक दबाव और रिएक्टर ऊंचाई के साथ प्रभावशीलता कारक के लिए प्रोफाइल की भविष्यवाणी की। इसके अलावा, तरल के खराब वितरण के प्रभाव का आकलन करना जो वास्तविक दुनिया में प्रासंगिक है; टीबीआर और आरएफआर के लिए 1-डी मॉडल को 2-डी ज्यामिति तक बढ़ा दिया गया था। 2-डी मॉडल ने रिएक्टर की ऊंचाई और व्यास के साथ प्रजातियों की एकाग्रता और तापमान प्रोफाइल पर रिएक्टर इनलेट पर तरल प्रवाह में परिवर्तन के प्रभाव का अनुकरण किया। रिएक्टर से आउटलेट स्ट्रीम में सल्फर सामग्री (पीपीएम) के संदर्भ में टीबीआर और आरएफआर के प्रदर्शन पर प्रभाव का विश्लेषण करने के लिए माल वितरण कारक एमएफ 0-0.6 की सीमा में भिन्न था। इसके अलावा, वर्तमान अध्ययन में टीबीआर के लिए विकसित 2-डी मॉडल का उपयोग वाणिज्यिक पैमाने टीबीआर में मापा अक्षीय और रेडियल तापमान प्रोफाइल के आधार पर खराब वितरण की सीमा और गर्म क्षेत्र के संभावित आकार को निर्धारित करने के लिए किया जा सकता है। आरएफआर के 2-डी मॉडल का उपयोग तरल वितरण के लिए अनुमत डिग्री या सीमा के साथ सुरक्षित और व्यवहार्य संचालन का आकलन करने के लिए किया जा सकता है।

इस शोध प्रबंध का अनूठा पहलू इस तथ्य में निहित है कि यह हाइड्रोप्रोसेसिंग के लिए तीन चरण रेडियल फ्लो रिएक्टर के लिए प्रायोगिक और सिमुलेशन अध्ययन पर ध्यान केंद्रित करने वाला प्रमुख शोध अध्ययन है।

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Nomenclature

A, B, C	constants used in correlation of pressure drop and dynamic liquid hold up
AARE	average absolute relative error, $AARE (\%) = \frac{1}{n} \sum_{i=1}^n \left 1 - \frac{y_{\text{predicted}}}{y_{\text{experimental}}} \right $
A_c	cross sectional area of reactor, m^2
a_{GL}	gas–liquid interfacial area, m^{-1}
a_{LS}	Liquid–solid interfacial area, m^{-1}
C	concentration in the liquid phase, mole/m^3
C_p	specific heat capacity, $J/(kg \text{ K})$
D, E	constants used in correlation of pressure drop and dynamic liquid hold up
D_{ax}	axial dispersion coefficient, m^2/s
d_p	particle diameter, m
d_{peq}	equivalent particle diameter, m
$d_{conduit}$	inner diameter of porous outer conduit, m
d_{dist}	outer diameter of gas distributor, m
$D_{e,k}$	Effective diffusivity = $\frac{D_k \varepsilon}{\text{Porosity}}$, m^2/s
D_k	Diffusivity of species 'k' in liquid, m^2/s
$d_{reactor}$	diameter of reactor, m
E	activation energy, $J/(kg \text{ K})$
H	Henry's coefficient, $MPa \text{ m}^3/\text{mole}$
ΔH	heat of reaction, $\text{kJ}/\text{Nm}^3 \text{ H}_2$ consumed
k_{int}	Intrinsic rate constant
K_L	gas liquid mass transfer coefficient, m/s

K_{LS}	liquid-solid mass transfer coefficient, m/s
L	radial bed length, $(d_{conduit}-d_{dist})/2$, m
M	Mass flow rate, kg/m ² s
N_{ax}	Number of CSTRs in axial direction
N_{rad}	Number of CSTRs in radial direction
N_{reG}	particle Reynolds number for gas, $\rho_G U_G d_{peq}/(\mu_G \epsilon)$
N_{reL}	particle Reynolds number for liquid, $\rho_L U_L d_{peq}/(\mu_L \epsilon)$
P	partial pressure, MPa
P_c	pressure in gas collection conduit, kPa
Pe	pecllet number, $U_L Z/D_{ax}$
$\left(\frac{\Delta P}{L}\right)$	pressure drop, kPa/m
Q	flow rate of liquid, m ³ /s
r	rate of reaction, mole/(m ³ s)
R	gas constant, J/mole K
r_1	outer radius of distributor, m
r_2	inner radius of porous conduit, m
S_P	surface area of particle, m ²
T	reactor temperature, K
U_G	gas superficial velocity, $Q_G/(\pi d_{dist} H)$, m/s
U_{Gi}	gas interstitial velocity, m/s
U_L	liquid superficial velocity, Q_L/A_R , m/s
v_0	gas volume under standard conditions

V_b	<i>volume of bed, m³</i>
V_P	<i>Volume of particle, m³</i>
V_P	<i>volume of particle, m³</i>
W_f	<i>wetting efficiency</i>
Z	<i>height of the reactor, m</i>

Subscripts

a	<i>Flow through bed</i>
b	<i>Bypass-weeping flow</i>
CH_4	<i>Methane</i>
G, g	<i>Gas</i>
H_2	<i>Hydrogen</i>
H_2S	<i>Hydrogen Sulfide</i>
L, l	<i>Liquid</i>
MA	<i>Mono aromatics</i>
NA	<i>Naphthenes</i>
O	<i>Olefins</i>
PA	<i>Poly aromatics</i>
q	<i>Quench</i>
S	<i>Sulfur</i>
SL	<i>Solid</i>
$Total$	<i>Total flow to reactor</i>

Greek letters

ε	<i>bed voidage</i>
ε_L	<i>dynamic liquid hold-up</i>
ε_T	<i>total liquid hold-up</i>
μ_G	<i>gas Viscosity, Pas</i>
μ_L	<i>liquid viscosity, Pas</i>
ρ_G	<i>gas density, kg/m³</i>
ρ_P	<i>catalyst particle density, 1200 kg/m³</i>
ρ_L	<i>liquid density, kg/m³</i>
φ	<i>sphericity</i>
τ_s	<i>space time, H/U_L , minutes</i>
τ_a	<i>mean residence time for flow through bed in weeping mode, s</i>
ϕ	<i>thiele Modulus</i>
η_{ef}	<i>effectiveness factor</i>
γ	<i>hydrogen stoichiometric coefficient for different reactions</i>
τ	<i>mean residence time, s</i>
τ_{avg}	<i>average of mean residence time, s</i>
σ	<i>surface tension</i>

Acronyms

<i>AGO</i>	<i>atmospheric gas oil</i>
<i>CSTR</i>	<i>constant stirred tank reactor</i>
<i>G/O</i>	<i>gas to oil ratio</i>

<i>LCO</i>	<i>light cycle oil</i>
<i>LHSV</i>	<i>liquid hourly space velocity</i>
<i>LPG</i>	<i>liquefied petroleum gas</i>
<i>MA</i>	<i>monoaromatics</i>
<i>MMTPA</i>	<i>million metric tons per annum</i>
<i>MT</i>	<i>mass transfer of species to liquid phase</i>
<i>NA</i>	<i>naphthenes</i>
<i>PFR</i>	<i>plug flow reactor</i>
<i>PNA</i>	<i>Poly nuclear aromatics</i>
<i>RFR</i>	<i>radial flow reactor</i>
<i>RTD</i>	<i>residence time distribution</i>
<i>TBR</i>	<i>trickle bed reactor</i>
<i>VGO</i>	<i>vacuum gas oil</i>