CHARACTERIZATION OF GAS–LIQUID FLOW THROUGH DISTRIBUTORS AND POROUS BEDS FOR CO–CURRENT DOWNFLOW PACKED BED REACTOR

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Characterization of Gas–Liquid Flow through Distributors and Porous Beds for Co–current Downflow Packed Bed Reactor

by

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Certificate

This is to certify that the thesis entitled **"Characterization of Gas–Liquid Flow through Distributors and Porous Beds for Co–current Downflow Packed Bed Reactor"** being submitted by **Ms. Ekta Ajit Jain** to the **Indian Institute of Technology Delhi, New Delhi** for the award of the degree of **Doctor of Philosophy** is a bonafide record of original research work carried out by her under our supervision in conformity with rules and regulations of the institute. The results contained in this thesis have not been submitted, in part or in full, to any other university or institute for the award of any degree or diploma.

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Abstract

Trickle bed reactors (TBRs) are widely used in the petrochemical and oil-industry, especially in hydro-treating and hydrocracking processes. With vehicular emission norms getting more stringent, there is a significant emphasis on development of high-performance catalysts and internal hardware for these reactors in order to produce clean fuels. In the co-current down-flow operations in these TBRs, gas and liquid, both enter the reactor from the top through a mixer, followed by a pre-distributor, and further, get re-distributed by principal gas-liquid distributors (arranged on the distributor tray). Of all the key factors affecting reactors' operational performance, the liquid distribution inside the bed is known to be crucial. However, the local liquid distribution and, subsequently, the hydrodynamics inside the bed is largely affected by the liquid distribution at the top of the packed bed. In the literature, while there are several studies on measurements or simulations of liquid distribution inside the bed, only a few investigations are available on distributor and tray efficiency. Also, to develop a detailed model for the flow through the entire distributor tray, a deeper understanding and quantification of the flow through individual units is necessary. Further, the development of a CFD methodology incorporating the gas-liquid distributor measurements is required to be able to predict the gas-liquid distribution inside the packed bed.

In the present work, the experimental investigations of liquid distribution generated by single units of standard chimney and bubble cap distributors are performed for a co-current downward flow of air and water with a *G/L* ratio widely used in the trickle bed industrial operations. The liquid holdup distribution is measured, and liquid flow morphology is analysed using in-house developed dual-tip voidage probes for air-water flow at the tray outlet. An Eulerian (3D, transient) two-fluid model is implemented with a suitable weighted drag formulation to simulate the flow that was comprising of multiple flow-regimes in a single flow-domain, and its predictions are compared with the measured liquid distribution, liquid height above the tray, and pressure drop. This is carried out in order to quantify the gas-liquid distribution through such individual units and to verify the CFD model, so that this information can be used readily to predict the flow through complete trays. Further, the analysis of flow through bubble cap distributor in combination with different liquid dispersion plates from the literature is carried out, experimentally and numerically. Also, the verified CFD model is can be used to carry out 2D transient simulations for diesel-hydrogen system under industrial operating conditions to develop highly efficient design of liquid distributor plates.

In addition to this, a methodology is developed to quantify the liquid distribution obtained through distributor trays taking into account the overlapping of liquid coverage spans between neighboring distributor units under industrial operating conditions, using two-phase Euler-Euler method. A comparative study of liquid distribution through trays with gas-liquid distributors of uniform and non-uniform (with artificially created positive-and negative-gradient) discharge pattern is also carried out for co-current downflow condition. Further, the predictions of liquid distribution obtained for aforementioned different configurations of distributor tray are used to obtain the gas-liquid distribution inside the bed for industrially relevant operating conditions. Such analysis and numerical simulations can be used to investigate the performance of new gas-liquid distributors, to validate the performance claims of existing distributor trays, and to assist in designing and optimizing new ones.

सहधारी अधोमुखी पैक्ड बेड रिऐक्टर में वितरकों एवं झरझरे बेड के माध्यम से गैस-तरल प्रवाह का विशेषीकरण

ट्रिकल बेड रिऐक्टर पेट्रोकेमिकल उत्पादों और तेल खनन एवं उत्पादन वाले उद्योगों में अत्यधिक उपयोग में लाये जाते हैं, ख़ासकर, हाइड्रोट्रीटिंग और हाइड्रोक्रैकिंग में। मोटर वाहनों के उत्सर्जन के मापदंड अधिक कठोर हो जाने के कारण इन रिएक्टरों में उच्च प्रदर्शन उत्प्रेरक और आतंरिक हार्डवेयर के विकास के लिए ठोस कदम उठाये जा रहे हैं। इन रिएक्टरों में अधोमुखी और सहधारा प्रवाह के संचालन में, गैस एवं तरल पदार्थ रिएक्टर के ऊपरी प्रवेशद्वार से अंदर आते हैं, फिर एक मिक्सर, और एक पूर्व-वितरक से गुज़र कर ट्रे में व्यवस्थित प्रधान वितरकों से होते हुए झरझरे बेड में प्रवेश करते हैं। इन रिएक्टरों के कार्य प्रदर्शन को प्रभावित करने वाले मुख्य कारणों में बेड के अंदर का तरल-वितरण बहुत ही महत्वपूर्ण है। हालांकि यह तरल-वितरण बेड के अंदर के स्थानीय वितरण और तरल गत्यात्मकता पर काफी हद तक निर्भर करता है। इससे सम्बंधित तकनीकी साहित्य में, बेड के आतंरिक तरल-वितरण के माप और सिम्युलेषन पर आधारित कई लेख हैं, परन्तु वितरकों और ट्रे की क्षमता पर बहुत कम अध्ययन हैं। इसके अतिरिक्त, पूर्ण वितरक ट्रे के द्वारा तरल-वितरण के गहन अध्ययन और परिमाणीकरण के लिए हरेक वितरक इकाई के संचालन का विस्तृत प्रारूप विकसित करना आवश्यक है। इसके साथ ही, एक सी.एफ.डी. क्रियाविधि विकसित करना आवश्यक है जिसमें गैस- तरल वितरण के माप के द्वारा झरझरे बेड के आतंरिक गैस-तरल वितरण की जानकारी मिल सके।

प्रस्तुत किये गए कार्य में, सम्बंधित उद्योगों के रिएक्टरों में प्रयोग होने वाली मानक चिमनी और बबल कैप की एकल इकाइयों के द्वारा हवा और पानी के एक निश्चित अनुपात के सहधारी अधोमुखी प्रवाह का प्रयोगात्मक विश्लेषण किया गया है। इस अध्ययन में अन्तः निर्मित द्विमुखी वॉइडेज-प्रोब का उपयोग कर के अधोद्वार पर हवा-पानी के आयतन-वितरण और प्रवाह-संरचना को जांचा गया है। एक ऑयलेरियन (३-डी, क्षणिक) द्वितरलीय प्रारूप को समायोज्य ड्रैग सूत्रीकरण के साथ ऐसा प्रवाह सिम्युलेट किया गया, जिसमें एक ही प्रवाह-आयाम में विभिन्न प्रवाह क्षेत्र हैं। इससे उत्पन्न आंकड़ों का मापे हुए तरल-वितरण, ट्रे के ऊपर तरल-स्तर और दबाव के साथ तुलनात्मक अध्ययन किया गया। इस प्रक्रिया से एकल वितरक इकाइयों के द्वारा संभव गैस-तरल वितरण को

परिमाणित किया गया, और सी.एफ.डी. प्रारूप को सत्यापित किया गया, ताकि पूर्ण ट्रे के वितरण-प्रदर्शन की जानकारी मिल सके। इसके आलावा, मानक बबल-कैप वितरक इकाई के साथ तकनीकी साहित्य में दिए गए विभिन्न डिस्पर्शन-प्लेटों द्वारा, प्रयोगात्मक और संख्यात्मक पद्धति से तरल-प्रवाह का विश्लेषण किया गया। इस सत्यापित सी.एफ.डी. प्रारूप से २-डी क्षणिक सिम्युलेषन के द्वारा उद्योग-सम्बन्धी परिचालन की स्थितियों में डीज़ल-हाइड्रोजन प्रवाह प्रणाली का अध्ययन कर के उच्च-प्रदर्शन डिस्पर्शन-प्लेट बनायी जा सकती है।

इसके अतिरिक्त, द्वितरलीय ऑयलेरियन प्रणाली द्वारा उद्योग-सम्बन्धी परिचालन की स्थितियों में सम्पूर्ण वितरक ट्रे की इकाइयों के तरल वितरण और उनके बीच के अतिव्यापन के संख्यात्मक विवरण के लिए एक कार्यप्रणाली विकसित की गयी। इसके साथ ही समान एवं असमान (कृत्रिम तरीके से निर्मित सकारात्मक और नकारात्मक ढाल) के वितरण प्रकारों वाली गैस-तरल वितरक इकाईयों का सहधारा और अधोमुखी प्रवाह के लिए तुलनात्मक अध्ययन किया गया। इसके बाद, ऊपर बताये गए अलग-अलग वितरण इकाईयों के माध्यम से उद्योग-सम्बन्धी परिचालन की स्थितियों में होने वाले गैस-तरल वितरण को पूर्वानुमानित किया गया। ऐसे विश्लेषण और संख्यात्मक अध्ययन से नए गैस-तरल वितरकों के प्रदर्शन को पूर्वानुमानित करने, मौजूदा इकाईयों के संचालन की जांच करने और नए वितरण इकाईयों के विन्यास को अनुकूलित बनाने में बहुत सहयोग मिलता है।

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Nomenclature

Notations

A	Face–area of a computational cell (m^2)
A_{total}	Total surface area of the flow plane (m^2)
C_D	Drag coefficient (–)
d_p	Characteristic length of the dispersed phase (m)
$E_{ö}$	Eötvös number (–)
F_{drag}	Drag force per unit volume $(kg/m^2.s^2)$
g	Gravitational acceleration (m/s^2)
G	Gas phase
G/L ratio	Gas/Liquid volumetric flow rate ratio (–)
K	Momentum exchange coefficient ($kg/m^3.s$)
L	Liquid phase
M	Inter–momentum exchange term ($kg/m^2.s^2$)
M_f	Maldistribution factor (–)
n	Total number of overlapping computational cells with same coordinates (–)
N	Total number of computational cells on the flow surface (–)
Q_i	Mass flow rate of liquid passing through cell i(kg/s)
Q_i'	Average mass flow rate of liquid through computational cell (kg/s)
$\mathrm{Q_G}$	Volumetric flow rate of gas (Nm^3/hr)
$\mathrm{Q_L}$	Volumetric flow rate of liquid (m^3/hr)
Q_{total}	Total mass flow rate of liquid passing through flow plane (kg/s)
Re	Reynolds number (–)
t	time for which the probe tips were covered by liquid
T	Total time of data acquisition
u,v,w	Instantaneous velocity in x, y and z–directions, respectively (m/s)
$u_{slip},v_{slip},w_{slip}$	Slip velocities in x, y and z–directions, respectively (m/s)
U	Instantaneous velocity (m/s)
V_{abs}	Absolute slip velocity (m/s)
V_G	Superficial velocity of gas (m/s)
V_L	Superficial velocity of liquid (m/s)
$W'=W/2$	Half the width of the test–rig (m)
x	Distance from the vertical–central axis of the test–rig (m)

Greek letters

α	Instantaneous phase holdup (–)
$\bar{\alpha}$	Time–averaged phase holdup (–)
k	Turbulent kinetic energy (m^2/s^2)
ε	Turbulent dissipation rate (m^2/s^3)
ρ	Density (kg/m^3)
μ	Dynamic viscosity ($kg/m/s$)
σ	Surface tension between the two phases (N/m)

Subscripts

a	Air
l, L	Liquid

v, G	Vapor (Gas phase)
w	Water
i	General index
n	number of times water droplet comes in contact with both the probe tips in total time *T*.

Abbreviations

BCWP	Bubble cap with test perforated plate
BCWOP	Bubble cap without plate (standard bubble cap)
BCSF	Bubble cap with rounded slots and angled–fins plate
BCSP	Bubble cap with spiral plate
CFD	Computational fluid dynamics
CWOP	Chimney without plate (standard chimney)
DHDS	Diesel hydrodesulfurisation
LED	Light–emitting diode
MFR	Mass flow rate
PG	Positive–gradient discharge pattern
TBR	Trickle bed reactor
NG	Negative–gradient discharge pattern
VOF	Volume of Fluid (method)