NUMERICAL INVESTIGATION OF LIQUID–LIQUID DISENGAGEMENT IN A BATCH AND CONTINUOUS GRAVITY SETTLER

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by

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Submitted

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

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Dedicated to my beloved

…Wife …

Certificate

This is to certify that the thesis entitled **"Numerical Investigation of Liquid–Liquid Disengagement in a Batch and Continuous Gravity Settler"** being submitted by **Mr. Saroj Kumar Panda** to the Indian Institute of Technology Delhi for the award of the degree of **Doctor of Philosophy** is a bonafide record of original research work carried out by him under my supervision in conformity with rules and regulations of the Institute. The results contained in this thesis have not been submitted elsewhere, either in part or in full, to any other University or Institute for the award of any degree or diploma.

Date:

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Saroj Kumar Panda

Abstract

The present research work is focused on the disengagement of liquid–liquid dispersion in a batch and continuous gravity settler using measurements and numerical simulations in OpenFOAM. Further, to developed an experimentally verified computational model that can predict the dynamics of such liquid–liquid flow in continuous and liquid phase disengagement in batch settler under different flow conditions (e.g. flow rate and fluid properties), internals (e.g. baffles, picket fence), different geometrical features (e.g. settler length, position of outlets, position of end–plate) and with different phase ratios.

Three–dimensional Eulerian–Eulerian (EE) simulations were performed by developing further the *twoPhaseEulerFoam* module of OpenFOAM. The effects of total liquid flow rate, drop diameter and organic phase density were investigated. The predicted effect of total liquid flow rate on dispersion–band thickness and organic phase volume fraction were compared with the measurements performed in a laboratory–scale continuous gravity settler. The drag coefficient correction factor was introduced in the drag model to account the drop swarms, led to improvements in the predictions of dispersion–band thickness and dispersed–phase volume fraction. The predicted results were found to be in a satisfactory agreement with the measurements. The observed difference in the measured and predicted results was due to the constant drop size considered in simulations.

The *twoPhaseEulerFoam* module was further used to perform EE simulations to study the effects of settler geometry (settling area, locations of aqueous phase outlet, position of end–plate) on the liquid–liquid separation in a continuous gravity settler. For a given flow rate of the dispersion, increase in the settler length (for a fixed width) led to increased settling area and also to increased residence time. It was found that, for settlers with L/W > 1.5, the insertion of picket fence did not improve the separation performance. However, for smaller L/W, the

insertion of picket fence led to a reduction in the dispersion–band thickness. The reduction in the aqueous outlet and end–plate height after certain level, no phase separation was achieved. A new correlation was developed for prediction of the dispersion–band thickness that successfully predicts the effects of dispersion flow rate, settling area, inlet baffle opening position, inlet phase ratio and the density ratio.

Further, the need of batch settling was studied by performing experiments in a laboratory–scale batch settler and later EE simulations were performed using the same geometry and dimension of the settler. The effects of organic (dispersed) to aqueous (continuous) phase ratio (α_a/α_b), impeller speed and phase properties were studied in detail. The predicted and measured dispersion–band thickness (position of active and passive interface), organic (dispersed) phase volume fraction were compared and a satisfactory agreement was obtained. As expected, high impeller speed generates smaller drop size that led to a longer time for phase separation. For a fixed impeller speed, decreasing the α_a/α_b ratio reduces the separation time (case of varying initial dispersion height). However, the phase separation time is increased significantly when the α_a/α_b in a constant initial dispersion height system is decreased. It was observed that due to high interfacial tension, kerosene–water system took longer time for phase separation compared to dodecane–nitric acid system.

The multi–fluid EE simulations (with and without PBM) were performed in the batch settler. The integration of a stand–alone population balance (PBM) code in the OpenFOAM CFD solver was carried out. The CFD+PBM solver (*multiPhaseCfdPbmFoam*) was used to perform 3D/laminar simulations in a batch settler to see the predictive capability of the model. For this purpose, the predicted active/passive interface and organic phase volume fraction distribution are compared with the measured data. The present work will be useful for the design of an optimal continuous settler configuration.

सार

वर्तमान शोध कार्य ओपनफोम में माप और संख्यात्मक सिमुलेशन का उपयोग करके एक बैच और निरंतर गुरुत्वाकर्षण निपटान में तरल-तरल फैलाव के विघटन पर केंद्रित है। इसके अलावा, एक प्रयोगात्मक रूप से सत्यापित कम्प्यूटेशनल मॉडल विकसित करने के लिए जो विभिन्न प्रवाह स्थितियों) जैसे प्रवाह दर और द्रव गुण (के तहत बैच सेटलर में निरंतर और तरल चरण विघटन में ऐसे तरल-तरल प्रवाह की गतिशीलता की भविष्यवाणी कर सकता है, आंतरिक) जैसे बफफलेस , पिकेट-फेंस (, विभिन्न ज्यामितीय विशेषताएं) जैसे सेटलर लेंथ, आउटलेट की स्थिति, अंत प्लेट की स्थिति (और विभिन्न चरण अनुपात के साथ।

ओपन फोम के *टूफेजयूलरफोम* मॉड्यूल से त्रि-आयामी यूलरियन-यूलरियन (ईई)सिमुलेशन किया गया तत्पश्चात कुल तरल प्रवाह दर, ड्रॉप व्यास और कार्बनिक चरण घनत्व के प्रभाव की जांच की गई। फैलाव-बैंड मोटाई और कार्बनिक चरण मात्रा अंश पर कुल तरल प्रवाह दर का अनुमानित प्रभाव एक प्रयोगशाला-पैमाने के निरंतर गुरुत्वाकर्षण निपटान में किए गए माप के साथ तुलना की गई। ड्रैग गुणांक सुधार कारक ड्रैग मॉडल में ड्रॉप स्वार्म्स को ध्यान में रखकर पेश किया गया था, जिससे डिस्पेरशन- बैंड मोटाई और डिस्पेर्सेड फेज वाले चरण मात्रा अंश की भविष्यवाणियों में सुधार हुआ और नतीजतन अनुमानित परिणाम माप के साथ संतोषजनक समझौते में पाए गए थे। मापा और अनुमानित परिणामों में पाए गए अंतर अनुकरण में निरंतर ड्रॉप आकार के कारण था।

तत्पश्चात *टूफेजयूलरफोम* मॉड्यूल का उपयोग निरंतर गुरुत्वाकर्षण निपटान में तरल-तरल पृथक्करण पर बसने वाले ज्यामिति (सेटलिंग एरिया, जलीय चरण आउटलेट के स्थान, अंत प्लेट की स्थिति) के प्रभावों का अध्ययन करने के लिए ईई सिमुलेशन करने के लिए किया गया । डिस्पेरशन की दी गई प्रवाह दर के लिए, बसने की लंबाई) एक निश्चित चौड़ाई के लिए (में वृद्धि के कारण निपटारे क्षेत्र में वृद्धि हुई और निवास के समय में वृद्धि हुई। यह पाया गया कि, एल / डब्ल्यू>1 . 5के साथ बसने वालों के लिए, पिकेट-फेंस के सम्मिलन में पृथक्करण प्रदर्शन में सुधार नहीं हुआ। हालांकि, छोटे एल / डब्ल्यू के लिए, पिकेट-फेंस के सम्मिलन ने डिस्पेरशन- बैंड मोटाई में कमी आई।

कुछ स्तर के बाद जलीय आउटलेट और अंत-प्लेट ऊंचाई में कमी, कोई चरण अलगाव हासिल नहीं किया गया। डिस्पेरशन- बैंड मोटाई की भविष्यवाणी के लिए एक नया सहसंबंध विकसित किया गया था जो डिस्पेरशन प्रवाह दर, क्षेत्र को व्यवस्थित करने, इनलेट बाफ्फ खोलने की स्थिति, इनलेट चरण अनुपात और घनत्व अनुपात के प्रभावों की सफलतापूर्वक भविष्यवाणी करता है। इसके अलावा, बैच निपटारे की आवश्यकता का प्रयोग प्रयोगशाला-स्केल बैच बसने

में प्रयोग करके किया गया था और बाद में ईई सिमुलेशन उसी ज्यामिति और बसने वाले के आयाम का उपयोग करके किया गया था। जलीय) निरंतर (चरण अनुपात) αa / αb), प्ररित करनेवाला गति और चरण गुणों के लिए कार्बनिक) डिस्पेर्सेड (का प्रभाव विस्तार से अध्ययन किया गया था। अनुमानित और मापा फैलाव-बैंड मोटाई) सक्रिय और निष्क्रिय इंटरफेस की स्थिति(, कार्बनिक) डिस्पेर्सेड (चरण मात्रा अंश की तुलना की गई और एक संतोषजनक समझौता प्राप्त किया गया। जैसा कि अपेक्षित था, उच्च प्रवेगक गति छोटे ड्रॉप आकार उत्पन्न करती है जिससे चरण अलग होने के लिए लंबा समय लगता है। एक निश्चित प्ररित करनेवाला गति के लिए, αa / αb अनुपात घटाने से पृथक्करण समय कम हो जाता है । हालांकि, चरण पृथक्करण समय में काफी वृद्धि हुई है जब निरंतर प्रारंभिक डिस्पेरशन ऊंचाई प्रणाली में αa / αb में कमी आई है। यह देखा गया था कि उच्च इंटरफेसियल तनाव के कारण, केरोसिन-जल प्रणाली में डोडकेन-नाइट्रिक एसिड प्रणाली की तुलना में चरण पृथक्करण के लिए अधिक समय लगा।

बैच बसने वाले में बहु-द्रव ईई सिमुलेशन(पीबीएम के साथ और बिना) (किए गए थे। ओपनएफएएम सीएफडी सॉल्वर में स्टैंड-अलोन आबादी बैलेंस) पीबीएम (कोड का एकीकरण किया गया था। सीएफडी + पीबीएम सॉल्वर) *मल्टीफेस सीएफडीपीबीएमएफओएम* (मॉडल की भविष्यवाणी क्षमता देखने के लिए बैच बसने वाले में 3 डी / लैमिनार सिमुलेशन करने के लिए प्रयोग किया जाता था। इस उद्देश्य के लिए, अनुमानित सक्रिय / निष्क्रिय इंटरफेस और कार्बनिक चरण मात्रा अंश वितरण मापा डेटा के साथ तुलना की जाती है। वर्तमान कार्य एक इष्टतम निरंतर निपटान विन्यास के डिजाइन के लिए उपयोगी होगा।

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Nomenclature

Symbols

A	Settling area, m^2
A_{CS}	Cross-sectional area of the settler, m^2
$b(v)$	Breakage frequency, s^{-1}
B_c	Birth term due to coalescence, m^3/s
B_b	Birth term due to breakage, m^3/s
C_1, C_2	Model parameters in turbulence model, (-)
C_1-C_{23}	Adjustable parameters, (-)
C'_1-C'_{24}	Adjustable parameters, (-)
C_D	Drag coefficient, (-)
C_L	Lift coefficient, (-)
C_{VM}	Virtual mass coefficient, (-)
d_B	Bubble diameter, m
d_d	Diameter of drop, μm
D_c	Death term due to coalescence, m^3/s
D_b	Death term due to breakage, m^3/s
$Eö$	Eotvos number, (-)
$f(x, t)$	Particle number distribution, (-)
F	Force, N
G, G_e	Turbulence generation, extra source of turbulence due to dispersed phase
g	Gravitational constant, m/s^2
h_i, h_f	Initial and critical film thickness, m

$H(x, t)$	Population balance equation source term
H	Dispersion band thickness (or dispersion height in batch settler), m
H_b	Baffle opening height, cm
H_t	Height of the end-plate, cm
k	Turbulent kinetic energy per unit mass, m^2/s^2
L	Settling length, m
L_i	i^{th} abscissa, m
$<l_w>$	Average distance between bubbles, m
l_e	Integral length scale of turbulence, m
m_k	k^{th} moment of bubble size distribution
$\vec{M}$	Interphase momentum exchange term, $kg/m^3.s$
N	Number of phases, (-)
P	Pressure, N/m^2
p	Drag correction factor, (-)
$P(v/v')$	Breakage probability term, m^{-3}
Pc	Coalescence efficiency
r, r_1, r_2	Bubble radius, m
R_a	Film radius, m
s	Source term due to coalescence and breakage
Q	Flow rate, l/hr
Q_t	Total flow rate, l/hr
Qd	Disperse phase flow rate, l/hr
Re	Reynolds number, (-)
t	Time, s

t_r	Residence time, s
u_{r1}, u_{r2}	Terminal rise velocity of bubbles, ms^{-1}
u_{rel}	Relative velocity between bubbles, ms^{-1}
U	Phase velocity, m/s
V_t	Settling velocity, m/s
V_1^{BOX}	Volume influenced by a wake m^3
V, V_1, V_2	Bubble volume m^3
w_i	i^{th} weight, (-)
x	Internal variables, m^3
x, y, z	Spatial coordinates (along width, height and depth, respectively), m
v	Velocity of particle, m^3

Greek Letters

α	Dispersed phase hold-up/volume fraction, (-)
β	Continuous phase hold-up/volume fraction, (-)
ε	Energy dissipation rate, m^2/s^3
μ	Viscosity, kg/m.s
μ_{eff}	Effective viscosity, kg/m.s
ν	Kinematic turbulent viscosity, m^2/s
ρ	Density, kg/m^3
σ	Interfacial tension, mN/m
$\bar{\bar{\tau}}$	Stress tensor, Pa
$\Gamma(x',x-x')$	Coalescence kernels, (-)
Υ_i	Fraction reassigned to nearby classes pivot, (-)

ξ_{12}	r_1/r_2
η	Test function, (-)

Superscripts

D, VM, L	Drag, virtual mass and lift force, respectively
c, b	Continuous phase
d, a	Dispersed phase

Subscripts

G or L	Gas or liquid phase
i	Interface
k	Reference to phase k
$lam,_{t,\,eff}$	Laminar, turbulent, effective