

# **Characterization of Pore- and Particle-Scale Single- and Two-Phase Flows in Porous Media**

by

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## Certificate

This is to certify that the thesis entitled “**Characterization of Pore- and Particle-Scale Single- and Two-Phase Flows in Porous Media**” being submitted by **Mr. Aniket S. Ambekar** 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 him under my 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

Single-phase turbulent flows through porous media is key to solid-catalyzed reactions such as methane-steam reforming, methanol or dimethyl ether synthesis, water-gas shift reactions, etc. Such a flow system is generally referred to as a packed bed reactor (PBR) in the literature. The bed-scale performance of the PBRs, i.e., reactant conversion, yield, pressure drop, etc., is significantly influenced by the particle-scale heat and mass transfer characteristics which in turn are determined by the particle-scale turbulence characteristics. Therefore, particle-resolved RANS simulations of a small section of PBR are extensively used to evaluate the effects of particle shape, to analyze particle-scale heat and mass transfer, etc. However, despite the extensive use of particle-resolved RANS simulations, the rigorous validation of the predictions of these simulations is lacking to a great extent. In the present work, the RANS simulations (with various two- and seven-equation turbulence models) and LES are performed. Their predictions are compared with a state-of-the-art DNS to identify turbulence model suitable for flow through packed beds. The reasons behind agreements/deviations of the predictions of RANS and LES simulations compared to the predictions of DNS are identified. Further, the DNS is utilized to identify the range of Reynolds number at which the flow transits from laminar to turbulent regime.

Other than single-phase flows, two-phase flows through porous media are also important to several applications. E.g., gas-liquid (G-L) flows in PBRs for hydro-desulphurization of fuels, CO<sub>2</sub> adsorption, hydrogenation, etc., and liquid-liquid (L-L) flows through reservoir rocks for oil recovery and ground-water remediation, etc. The performance of all the above processes is a strong function of particle-/pore-scale flow phenomenon. The particle-/pore-scale two-phase flow dynamics is influenced by fluid-fluid (i.e., interfacial tension, viscosity/density ratio, etc.) and fluid-solid (governed by wettability) interactions as well as the

media structure (characterized by particle size/shape, pore topology/size distribution, and other structural heterogeneities), other than operating conditions. In the present work, both G-L and L-L flows through 3D pore-/particle-resolved mediums are investigated using the algebraic and geometric Volume-of-Fluid (VOF) simulations implemented in opensource CFD code OpenFOAM and commercial flow solver Ansys FLUENT, respectively. Before proceeding with the two-phase flow through realistic mediums (created using Rigid Body Simulations), the predictions of VOF simulations are rigorously validated with the aid of measurements (performed by us as well as other researchers).

With respect to G-L flow through packed beds the dynamics of liquid spreading in gas filled domain is investigated. With aid of dimensionless numbers [Ohnesorge, Weber, and  $AB_i$  (proposed in the present work)], the relative magnitude of governing forces at various stages of liquid spreading influenced weakly, moderately, and strongly by gravitational force is studied. The relationship between dimensionless numbers, lateral extent of liquid spreading, and void-scale flow behavior is established and shown in the form of a regime map. Concerning L-L flows, the effects of waterflooding velocity, interfacial tension (i.e., Capillary number ‘ $Ca$ ’) and wettability on oil recovery, ganglia size distribution and their location, and forces acting on the trapped ganglia are investigated. To develop fundamental understating of the flow physics the pore-scale oil recovery mechanisms as a function of forces acting on the trapped ganglia are investigated. Further, the relationship between pore-scale mechanisms,  $Ca$ , wettability, and oil recovery is established. Finally, a regime map displaying the pore-scale mechanism as a function of  $Ca$  and wettability is proposed.

## संक्षेप

ठोस-उत्प्रेरित प्रतिक्रिया का मुख्य आधार छिद्रयुक्त माध्यम में सिंगल फेस टर्बल्यूंट बहाव है, जैसे-मीथेन-भाप रिफॉर्मिंग, मेथेनॉल अथवा डाईमेथिल इथर का संश्लेषण, जल-वायु शिफ्ट प्रतिक्रिया इत्यादि। वैज्ञानिक साहित्य के अनुसार इसे पैकड बेड रिएक्टर कहा जाता है। पैकड बेड रिएक्टर का बेड स्तर का निष्पादन जैसे कि अभिकारक का रूपांतरण, निर्णायक पैदावार, दबाव आदि है, कण-स्तर के ग्रीष्म अथवा द्रव्यमान अंतरण पर जो कि कण-स्तर के टर्बुलेंस चित्रण से तय होता है को अर्थपूर्ण प्रभावित करता है। इसलिए पैकड बेड रिएक्टर के छोटे से हिस्से का, बड़े पैमाने पर, कण-स्थिर आरएएनएस सिमुलेशन में कण के आकार का प्रभाव, कण के ग्रीष्म अथवा द्रव्यमान अंतरण का स्तर आंकने में प्रयोग होता है परंतु कण-स्थिर आरएएनएस सिमुलेशन के अत्यधिक प्रयोग के बावजूद भी किसी दृढ़ विधिमान्यकरण अथवा आगमकथन पर पहुंचना थोड़ा कठिन है। प्रस्तुत कार्य में आरएएनएस सिमुलेशन (दो एवं सात समीकरण वाले टर्बुलेंस प्रतिमान) और एलईएस कार्यवानवित हुए हैं। उनके कथन की अत्याधुनिक डीएनएस से तुलना की गई है ताकि हम उस टर्बुलेंस प्रतिमान को तादात्म्य स्थापित कर सकें जो पैकड बेड बहाव के लिए उपयुक्त है। आरएएनएस एवम एलईएस के अनुबंध/विचलन के कथन के तर्क-वितर्क की डीएनएस के आगमकथन से तुलना की गई है, तदपश्चात डीएनएस को रेनॉल्ड्स नंबर की सीमा निर्धारित करने में प्रयोग किया है जिससे की लेमिनार से टर्बुलेंट रिजाइम का बहाव निर्धारित हो।

सिंगल फेस बहाव के अलावा, दो-फेस बहाव भी छिद्र युक्त माध्यम के लिए विविध प्रयोगात्मक महत्ता रखता है, जैसे कि पैकड बेड रिएक्टर में गैस-तरल बहाव में ईंधन का हाइड्रो-डीसल्फुराइजेशन, कार्बन डाइऑक्साइड का अधिशोषण, हाइड्रोजनीकरण आदि और तरल-तरल बहाव का चट्टान रिजर्वायर के अपरोक्ष में तेल-प्राप्त करने की क्रिया, भूजल निवारण आदि-उपयुक्त सभी प्रक्रियाओं का निष्पादन कण/छिद्र स्तर बहाव तथ्य का दृढ़ कृत्य है। कण/छिद्रस्तर का दो फेस बहाव का संचालन तरल-तरल अथवा ठोस तरल की परस्पर क्रिया से, माध्यम की संरचना से, परिचालन स्थिति में प्रभावित होता है। प्रस्तुत कार्य

में दोनों गैस-तरल एवम तरल-तरल बहाव का त्रिविम दृश्यन छिद्र/कण-स्तर के माध्यम से अनुसंधान किया गया है जिसमें एलजेब्राइक एवम ज्योमेट्रिक वॉल्यूम ऑफ फ्लूइड सिमुलेशन को मुक्त स्रोत सीएफडी कोड, ओपनफोम और व्यवसायिक बहाव सॉल्वर एंसिस फ्लूट कार्यान्वित हुए हैं। वॉल्यूम ऑफ फ्लूइड के आगमकथन को आगे बढ़ने से पूर्व दो-फेस बहाव के वास्तविक माध्यम को माप की सहायता से दृढ़ता से सत्यापित किया गया है।

जो तरल गैस प्रभावित क्षेत्र में फैल रहा है, उसका गैस-तरल बहाव का पैकड बेड माध्यम के संबंध से अनुसंधान हुआ है। आयामहीन संख्या की सहायता से तरलता विभिन्न चरणों में शासी बाल द्वारा विस्तृत प्राचल श्रृंखला में कैसे प्रभावित होती है, इसका अध्ययन किया गया है। एक रिजाइम मानचित्र की सहायता से आयामहीन संख्या का संबंध तरलता के पार्श्व विस्तार से एवम वॉइड-स्तर बहाव की गतिविधि से दर्शाया गया है। तरल-तरल बहाव से संबंधित - वॉटर फ्लॉडिंग वेग का प्रभाव, उक्त तलों के बीच का खिंचाव और तेल रिकवरी की नमनियता, गंगलिया का आकार वितरण और उनकी अवस्थिति और ट्रैप्ड गंगलिया पर जो बल काम कर रहे हैं, उनका अनुसंधान किया गया है। भौतिक बहाव की मौलिक समझ को विकसित करने के लिए छिद्र-स्तर तेल रिकवरी क्रिया-विधि ट्रैप्ड गंगलिया का सक्रिय बल कृत्य है, इस पर अध्ययन किया गया है। आगे छिद्र-स्तर क्रिया विधि नमनियता और तेल रिकवरी के बीच संबंध स्थापित किया गया है। अंततः एक रिजाइम मानचित्र जो छिद्र स्तर की क्रिया-विधि, कैपिलरी संख्या एवम नमनियता का कृत्य है, इसे प्रस्तावित किया गया है।

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