CHARACTERIZATION OF DYNAMICS OF BINARY GAS-SOLID FLOWS AND COAL GASIFICATION IN FLUIDIZED BEDS: HIGH-SPEED IMAGING MEASUREMENTS AND CFD SIMULATIONS

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by

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Submitted

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Certificate

This is to certify that the thesis entitled **"Characterization of Dynamics of Binary Gas-Solid Flows and Coal Gasification in Fluidized Beds: High-Speed Imaging Measurements and CFD Simulations"** is being submitted by **Ms. Sirisha Parvathaneni** 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 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

Gas-solids fluidized beds are widely used in several industrial processes like coal/biomass gasification and/or combustion, catalytic polymerization, etc. These industrial processes often involve fluidizing/defluidizing of a mixture of particles that differ in size or density or shape, e.g., fluidizing of coal/biomass and inerts in the gasification process, and defluidizing of different-sized polymer particles in catalytic polymerization. Therefore, the performance of these industrial processes is predominantly influenced by the spatial distribution of solid phases which is primarily governed by the local bubbling behavior. Depending on the particle size/density ratios and operating superficial gas velocities (U_G), the bubble carries lesser dense/bigger size particles with it leading to segregation of higher dense/smaller size particles. Such different segregation and mixing mechanisms should be predicted accurately by the CFD models. Such models can be further extended to simulate the industrial-scale fluidized bed reactors. Since the flow is inherently unsteady the CFD models should be validated with time- and space-resolved measurements.

In the present work, the dynamics of the binary gas-solids flows with particles differing in density or size or both in a pseudo-2D rectangular fluidized bed is characterized using high-speed imaging measurements. The bubbling characteristics were controlled using three different modes of air injection: uniform, two-jet, and single-jet distributors under the same U_G. The local individual phase area fraction fluctuations of all three phases (air and two solids) were measured. These measurements were further used to quantify the effects of particle size/density ratio, bed composition, mode of air injection, and U_G on the bubbling characteristics (bubble size distribution and local bubbling frequency) and eventually on the dynamics of segregation/ mixing. These measurements form a crucial database for the validation of Eulerian multi-fluid and CFD-DEM models which is the other objective of the present work.

The multi-fluid Eulerian simulations were performed for binary mixtures varying in size and/or density ratios, bed composition, U_G, and modes of gas injection. The results show that the models/parameters (gas-solid drag, solids frictional pressure, and specularity coefficient) that predicted the bubbling/spouting behavior of corresponding unary gas-solids flows correctly, predicted the bubbling/spouting behavior and dynamics of segregation of binary gas-solids flow accurately. Further, the roles of different forces (gas-particle drag, particle-particle drag, and solids viscosities) on the kinetic energies of the solid phases and ultimately on certain segregation and mixing mechanisms were quantified. The present work provides a detailed understanding of the flow physics for different operating parameters i.e., mode of gas injection, particle size/density ratios, bed composition, and U_G on local spouting/bubbling behavior and eventually on dynamics of segregation/mixing. Furthermore, in the coal gasification process, the effect of different local bubbling behaviors on the segregation/mixing of coal and inert solid phases and ultimately on reaction mechanisms, syngas composition, and syngas quality was quantified.

सार

गैस-ठोस द्रवित बेड का व्यापक रूप से कई औद्योगिक प्रक्रियाओं जैसे कोयला / बायोमास गैसीकरण और / या दहन, उत्प्रेरक पोलीमराइजेशन, आदि में उपयोग किया जाता है। इन औद्योगिक प्रक्रियाओं में अक्सर कणों के मिश्रण का द्रवीकरण / डिफ्लुइडाइजिंग शामिल होता है जो आकार या घनत्व या आकार में भिन्न होते हैं, उदा। , गैसीकरण प्रक्रिया में कोयले/बायोमास और अक्रिय का द्रवीकरण, और उत्प्रेरक पोलीमराइजेशन में विभिन्न आकार के बहुलक कणों का द्रवीकरण। इसलिए, इन औद्योगिक प्रक्रियाओं का प्रदर्शन मुख्य रूप से ठोस चरणों के स्थानिक वितरण से प्रभावित होता है जो मुख्य रूप से स्थानीय बुदबुदाती व्यवहार द्वारा नियंत्रित होता है। कण आकार/घनत्व अनुपात और ऑपरेटिंग सतही गैस वेग (यूजी) के आधार पर, बुलबुले में कम घने/बड़े आकार के कण होते हैं जिससे उच्च घने/छोटे आकार के कणों का पृथक्करण होता है। सीएफडी मॉडल द्वारा इस तरह के अलग-अलग अलगाव और मिश्रण तंत्र की सटीक भविष्यवाणी की जानी चाहिए। औद्योगिक पैमाने पर द्रवीकृत बिस्तर रिएक्टरों का अनुकरण करने के लिए इस तरह के मॉडल को और बढ़ाया जा सकता है। चूंकि प्रवाह स्वाभाविक रूप से अस्थिर है, इसलिए सीएफडी मॉडल को समय और स्थान-समाधान माप के साथ मान्य किया जाना चाहिए।

वर्तमान कार्य में, बाइनरी गैस-ठोस की गतिशीलता घनत्व या आकार में भिन्न कणों के साथ बहती है या दोनों एक छद्म -2 डी आयताकार द्रवित बिस्तर में उच्च गति इमेजिंग माप का उपयोग करने की विशेषता है। बुदबुदाती विशेषताओं को वायु इंजेक्शन के तीन अलग-अलग तरीकों का उपयोग करके नियंत्रित किया गया था: एक ही यूजी के तहत वर्दी, दो-जेट और एकल-जेट वितरक। सभी तीन चरणों (वायु और दो ठोस) के स्थानीय व्यक्तिगत चरण क्षेत्र अंश के उतार-चढ़ाव को मापा गया। इन मापों का उपयोग कण आकार/घनत्व अनुपात, बिस्तर संरचना, वायु इंजेक्शन के तरीके, और बुदबुदाहट विशेषताओं (बुलबुला आकार वितरण और स्थानीय बुदबुदाहट आवृत्ति) पर और अंततः अलगाव/मिश्रण की गतिशीलता पर प्रभाव को मापने के लिए किया गया था। ये माप यूलेरियन मल्टी-फ्लुइड और

सीएफडी-डीईएम मॉडल के सत्यापन के लिए एक महत्वपूर्ण डेटाबेस बनाते हैं जो वर्तमान कार्य का अन्य उद्देश्य है।

बहु-द्रव यूलेरियन सिमुलेशन आकार और / या घनत्व अनुपात, बिस्तर संरचना, यूजी, और गैस इंजेक्शन के तरीकों में भिन्नता वाले बाइनरी मिश्रण के लिए किए गए थे। परिणाम बताते हैं कि मॉडल/पैरामीटर (गैस-सॉलिड ड्रैग, सॉलिड फ्रिक्शनल प्रेशर, और स्पेक्युलरिटी गुणांक) जिसने संबंधित यूनरी गैस-सॉलिड्स के बुदबुदाहट/स्पाउटिंग व्यवहार की भविष्यवाणी की थी, सही ढंग से बहती है, बुदबुदाती/स्पाउटिंग व्यवहार और बाइनरी के अलगाव की गतिशीलता की भविष्यवाणी की थी। गैस-ठोस प्रवाह सही ढंग से। इसके अलावा, ठोस चरणों की गतिज ऊर्जाओं पर और अंततः कुछ अलगाव और मिश्रण तंत्र पर विभिन्न बलों (गैस-कण ड्रैग, कण-कण ड्रैग, और ठोस चिपचिपाहट) की भूमिकाएं निर्धारित की गईं। वर्तमान कार्य विभिन्न ऑपरेटिंग मापदंडों के लिए प्रवाह भौतिकी की एक विस्तृत समझ प्रदान करता है, अर्थात गैस इंजेक्शन का तरीका, कण आकार / घनत्व अनुपात, बिस्तर संरचना, और स्थानीय स्पाउटिंग / बबलिंग व्यवहार पर यूजी और अंततः अलगाव / मिश्रण की गतिशीलता पर। इसके अलावा, कोयला गैसीकरण प्रक्रिया में, कोयले और अक्रिय ठोस चरणों के पृथक्करण/मिश्रण पर और अंततः प्रतिक्रिया तंत्र, सिनगैस संरचना और सिनगैस गुणवत्ता पर विभिन्न स्थानीय बुदबुदाहट व्यवहारों का प्रभाव निर्धारित किया गया था।

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Nomenclature

Notations

U_{mf}	minimum fluidization velocity (m/s)
U_{mb}	minimum bubbling velocity (m/s)
U_{fc}	critical fluidization velocity (m/s)
U_{if}	initial fluidization velocity (m/s)
U_{ff}	final fluidization velocity (m/s)
U_G	superficial gas velocity (m/s)
d_{pr}	size ratio (-)
d_s	diameter of particle (m)
d_b	diameter of bubble (cm)
h_s	dispersion height of solid (m)
W	width of the bed (m)
$U_{G,injection}$	injection ags velocity (m/s)
H_b	initial static bed height (m)
H_d	heterogeneity index (-)
$x_{flotsam}$	mass fraction of flotsam (-)
K_{fri}	coefficient of friction for long-term particle frictional contacts (-)
C_{fri}	coefficient of friction for short-term particle frictional contacts (-)
$\overrightarrow{U_g}$	velocity of gas phase (m/s)
$\overrightarrow{U_{s_\iota}}$	velocity of solid phase (m/s)
$\overrightarrow{U_{s_\iota w}}$	velocity of ith solid phase near the wall (m/s)
P_g	shared gas phase pressure (pa)
P_s^t	solid phase pressure (Pa)
p_s	solids pressure due to kinetic and collisional effects (pa)
$P_{s,f}$	solids frictional pressure (pa)
$e_{s,w}$	particle-wall normal restitution coefficient (-)
e_{ss}	particle-particle restitution coefficient (-)
$g_{0,ss}$	radial distribution function (-)
d_s	diameter of solid phase (m)
C_D	drag coefficient (-)
H_d	heterogeneity index (-)
S_{sg}	mass source term (kg/m^{2}s)
Mw_{char}	molecular weight of char (kg/kmol)
$Mw_{g,i}$	molecular weight of species ‘i’ in gas mixture-gas (kg/kmol)
$Y_{g,i}$	species in gas phase (-)
$Y_{s,i}$	species in solid phase (-)
$R_{s,i}$	heterogenous reaction rate (kmol/m^{3}s)

$R_{g,i}$	homogenous reaction rate (kmol/m^{3}s)
T	temperature of the gas phase (k)
R	universal gas constant (J/kmol.K)
$\bar{g}$	gravity acceleration (m/s^2)
$\bar{\bar{I}}$	identity matrix
I_{2D}	second order stress tensor (s^{-1})
H_g	enthalpy of gas phase (J/kg)
H_{s_i}	enthalpy of ith solid phase (J/kg)
H_i	enthalpy of species 'i' (J/kg)
$C_{p,i}$	specific heat of species 'i' (J/kg.K)
$\Delta H_{f,i}$	heat of formation (J/kg)
h_{gs_i}	heat transfer coefficient between gas and ith solid phase (W/m^{2}K)
$J_{g,i}$	diffusion flux of species 'i' (1/m^{2}s)
$D_{i,j}$	binary mass diffusion coefficient (m^2/s)
Nu_s	Nusselt number (-)
Re_s	Reynolds number of solid phase (-)
Sc_t	Schmidt number (-)

Greek symbols

$\emptyset_s$	sphericity (-)
σ^2	variance (-)
σ_s^2	variance of a phase when the bed is completely segregated (-)
σ_M^2	variance of a phase when the bed is completely mixed (-)
α_g	volume fraction of gas-phase (-)
α_{s_i}	volume fraction of ith solid phase (-)
α_{s_k}	volume fraction of ith solid phase (-)
$\alpha_{s,min}$	minimum frictional packing limit (-)
$\alpha_{s,max}$	maximum frictional packing limit (-)
ρ_{pr}	diameter ratio (-)
ρ_g	density of gas-phase (kg/m^3)
ρ_{s_i}	density of ith solid phase (kg/m^3)
$\rho_{s,i}$	density of species 'i' in mixture-solid (kg/kmol)
$\bar{\bar{\tau}}_g$	gas phase stress tensor (pa)
$\bar{\bar{\tau}}_{s_i}$	ith solid phase stress tensor (pa)
$\bar{\bar{\tau}}_{s_i,w}$	wall shear stress of ith solid phase (pa)
β_{gs}	momentum exchange coefficient between gas phase and solid phase (kg/m^{3}s)
$\beta_{s_i s_k}$	momentum exchange coefficient between ith solid phase to kth solid phase (kg/m^{3}s)
β_{pec}	peculiar particle–particle drag coefficient (kg/m^{3}s)
β_{hyd}	fluid-dynamic particle–particle drag coefficient (kg/m^{3}s)
β_{fri}	frictional particle–particle drag coefficient (kg/m^{3}s)

μ_s	viscosity of solid phase (pa.s)
μ_g or μ_{gl}	viscosity of gas phase (pa.s)
μ_{gt}	turbulent viscosity of gas phase (pa.s)
$\mu_{s,col}$	collisional viscosity of solid phase (pa.s)
$\mu_{s,kin}$	kinetic viscosity of solid phase (pa.s)
$\mu_{s,fr}$	frictional viscosity of solid phase (pa.s)
λ_{sb}	bulk viscosity of solid phase (pa.s)
λ_s	thermal conductivity of gas phase (W/m.K)
λ_g	thermal conductivity of gas phase (W/m.K)
$\lambda_{s,i}$	thermal conductivity of species 'i' in solid phase (W/m.K)
$\lambda_{g,i}$	thermal conductivity of species 'i' gas phase (W/m.K)
Θ_s	granular temperature of solid phase (m^2/s^2)
κ_Θ	diffusional coefficient of granular temperature of solid phase (kg/ms)
γ_Θ	collisional dissipation of energy of solid phase (kg/ms^3)
γ_{char}	stoichiometric coefficient (-)
ϕ	particle-wall tangential restitution coefficient also termed as specularity coefficient (-)
φ	switch function
κ	turbulent kinetic energy (m^2/s^2)
ε	rate of dissipation of turbulent kinetic energy (m^2/s^3)

Acronyms

CFD	computational fluid dynamics
DEM	discrete element method
ECT	electrical capacitance tomography
TFM	two fluid model
MFM	multi fluid model