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Comparison of turbulence models for bubble column reactors

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HIGHLIGHTS

- CFD simulations of a bubble column are done by using k-ε model, RSM and LES models.
- Modeling approach is developed for conservation equations of k, ε and RSM.
- True k-ε model and true RSM are compared against the std. k-ε model and RSM as well as against LES model.
- The severity of modeling assumptions and their validity for two-phase flow is discussed in great details.

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ABSTRACT

Though bubble column reactors are widely used in industry, the present design practice is still closer to an art than a desired state of science because of the complexity of its fluid mechanics. The empiricism can be reduced by understanding detailed flow pattern, turbulence characteristics and turbulent structures and their effects on the performance such as mixing and axial mixing in both the phases and rate of heat and mass transfer. For this purpose, in the present work, CFD simulations have been undertaken by using standard k-ε, RSM and LES turbulence models. The cylindrical column having a computational height of $H_D = 900$ mm with inside diameter of $D = 150$ mm was employed as a bubble column operated at three superficial gas velocities (20, 40 and 100 mm/s). The instantaneous three dimensional velocity field is obtained by means of two phase Eulerian-Eulerian Large Eddy Simulations (LES). The conservation equations for turbulent kinetic energy (k) and the turbulent energy dissipation rate (ε) have been derived from the two fluid governing equations using the Reynolds averaging procedure. This enabled accurate estimation of convective transport, diffusive transport, turbulent transport, production and dissipation of k and ε. These estimations have been compared with the modelled terms of the standard k-ε and Reynolds stress models. The difference in values gives an idea about the severity of assumptions made in these models. An attempt has been made to bring out the implications of simplifying assumptions.

1. Introduction

The current design and scale-up procedures for multiphase systems (flow systems, reactors, separation equipment, etc.) need long commercialization time for generating confidence through the extensive data generation in the laboratory, pilot and demonstration scales. It also results into high capital as well as operating expenditure, long start-up and shut down times, etc. The genesis of these drawbacks lie in the empiricism which originates from the lack of knowledge of fluid mechanics and its relationship with the design objectives. In order to improve the lack of understanding, over the past 50 years, continuous efforts are being made using Experimental Fluid Dynamics (EFD) and Computational Fluid Dynamics (CFD). The progress in CFD has been remarkable considering the complexity of the three dimensional turbulent multiphase flows. This has been made possible by the combined developments in numerical methods and computational speed. However, substantial additional work is needed in understanding the physics of turbulence (of multiphase systems) so that equations of conservation of mass, momentum, energy and scalar (enthalpy, tracer, reactant, etc.) can be solved with the first principles. Therefore, with the current status of knowledge, a good number of assumptions are needed in the low order models such as k-ε and RSM. The standard k-ε model has performed satisfactory in many flows, but the applicability of this model is limited due to the uncertainties involved (because of simplifying assumptions) in the modeling of turbulence production and dissipation, turbulent convective transport, etc. (discussed later). It is known that the

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Nomenclature

C_μ	closure relationship in k-ε model: turbulent parameter that relates turbulent viscosity with k and ε
$C_{\mu,G}$	constant of Sato-Sekoguchi model
$C_{\varepsilon 1}$	model parameter in ε equation
$C_{\varepsilon 2}$	model parameter in ε equation
C_D	drag coefficient
C_{ke}	constant in Eq. (8)
C_L	lift coefficient
C_{R1}	constant in Eq. (27)
C_S	Smagorinsky coefficient
C_{TD}	turbulent dispersion constant in Eq. (24)
C_{VM}	virtual mass coefficient
D	column diameter, m
d_B	bubble diameter, m
E	energy available for bubble generated turbulence, W
e_D	rate of pressure energy in bubble column, W
E_D	total energy dissipation rate in bubble column, W
E_i	energy input rate to the bubble column, W
E_O	energy output rate with gas, W
E_N	net energy input rate to the bubble column, W
f_B	buoyancy force
f_D	drag force
f_G	gravity force
F_i	interphase force due to drag and lift
G_{KL}	rate of production of turbulent kinetic energy from mean kinetic energy, W m^{-3}
g	acceleration due to gravity, m s^{-2}
H_D	height of gas-liquid dispersion, m
K_{GL}	constant in Eq. (8) for the estimation of bubble generated turbulence
k	turbulent kinetic energy, $m^2\ s^{-2}$
l	length scale
P	pressure, Pa
P_{ij}	production of stress in Eq. (27)
$\bar{P}$	mean component of pressure, Pa
P'	fluctuating pressure, Pa
R	radius of column, m
r	radial distance from the centerline, m
S_{ij}	characteristic strain tensor in Smagorinsky model
S_k	source term in the conservation equation for k for bubble generated turbulence, $m^{-1}\ s^{-2}$
S_ε	source term in conservation equation for ε
u_i, u_j, u_k	three components of liquid velocity, m s^{-1}
$\bar{u}_i, \bar{u}_j, \bar{u}_k$	three mean components of liquid velocity, m s^{-1}
u'_i, u'_j, u'_k, u'_m	three fluctuating components of liquid velocity, m s^{-1}
V_L	superficial liquid velocity, m s^{-1}
V_G	superficial gas velocity, m s^{-1}
V_S	slip velocity, m s^{-1}
v_B	volume of bubble, m^{-3}
v_i	three components of gas velocity, m s^{-1}
z	axial location, m

Greek letters

δ_{ij}	Kronecker delta
ε	turbulent energy dissipation rate, $m^2\ s^{-3}$
$\in_G$	fractional gas hold-up
$\in_L$	fractional liquid hold-up
$\bar{\in}_G$	mean gas hold-up
$\bar{\in}_L$	mean liquid hold-up
$\in'_G$	fluctuating gas hold-up
$\in'_L$	fluctuating liquid hold-up
μ	molecular viscosity, kg $m^{-1}\ s^{-1}$
$\mu_{eff,l}$	effective viscosity, kg $m^{-1}\ s^{-1}$
v	kinematic viscosity, $m^2\ s^{-1}$
v_t	eddy or turbulent diffusivity, $m^2\ s^{-1}$
ρ_G	gas density, kg m^{-3}
ρ_L	liquid density, kg m^{-3}
σ_k	turbulence parameter in k equation
σ_ε	turbulence parameter in ε equation
τ_{ij}	Reynolds stress, Pa
τ_P	characteristic time for bubble generated turbulence in Eq. (25)
ϕ	instantaneous properties such as $u_i, u_j, u_k, \in_L, \in_G, P$
$\bar{\phi}$	mean properties such as $\bar{u}_i, \bar{u}_j, \bar{u}_k, \bar{\in}_L, \bar{\in}_G, \bar{P}$
ϕ'	fluctuating properties such as $u'_i, u'_j, u'_k, \in'_L, \in'_G, P'$
ω	vorticity, s^{-1}
Δ	filter width in LES model
Δt	time step, s

Subscripts

1	Direction along X-axis
2	Direction along Y-axis
3	Direction along Z-axis
G	Gas phase
L	Liquid phase

Superscripts

′	Fluctuating variable

Averages

<>	Reynolds averaging
Overbar	Time averaged variable

Abbreviations

BIT	bubble induced turbulence
CEL	CFX expression language
CGNS	CFD general notation system format
NaN	not a number
RANS	Reynolds averaged Navier-Stoke
SD	Standard deviation

number of assumptions decreases as the order of turbulence models becomes higher in the sequence of Reynolds Stress Model (RSM), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS). Though the accuracy of predictions increases from k-ε to DNS, the demand on computational time increases by orders of magnitude. In fact, the DNS simulation of even moderate size multiphase equipment is possible only at places of super computational facilities. Therefore, it was thought desirable to compare understand the k-ε, RSM and LES approaches for gas-liquid bubble columns in terms of quantitative values of errors versus the different simplifying assumptions.

At this stage, it may be pointed out that k-ε and RSM approaches are based on RANS and LES is another completely different approach. RANS is based on Reynolds-average that transforms a chaotic field (that is obtained by solving the governing equations with DNS) into a non-chaotic field. LES instead, by filtering the equations, takes a chaotic field and transforms it into another chaotic field, in which some scales are filtered out.

The conservation equations for k, ε and Reynolds stress consist of convective transport, diffusive transport, turbulent transport, production and dissipation. These terms are derived from the equations of continuity and motion (through Reynolds averaging