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Modeling of Pressure Drop in a Catalytic Distillation Column With Bale Packing for Tertiary Butyl Alcohol production

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Abstract: The computational fluid dynamics (CFD) technique was used to investigate the aerodynamics of catalytic Bale packing (used for the synthesis of tertiary butyl alcohol (TBA) in a pilot scale catalytic distillation column) using commercial CFD software Fluent 6.1. The global porosity of catalytic bales was considered instead of geometrical features for 2D simplification. The pressure drop simulations were performed and the results compared with the experimental studies. The CFD pressure drop results achieved by combination of power law and polynomial model were found to be in good agreement with the experimental data. The pressure drop results show that wall wipers reduce the pressure drop in the column significantly by increasing gas radial velocity and lower the gas axial velocity.

Keywords: CFD, User defined Scalars, Bales packing, and Pressure drop modeling

I. INTRODUCTION

Computational fluid dynamics (CFD) is a valuable aid to understand flow dynamics and mass transfer properties of catalyst. The packing plays a crucial role to achieve better separation and product yield [1]. Some of the limitations encountered experimentally can be overcome by CFD techniques. Harris et al [2] and Dudokovic[3] present a good overview on the capabilities of CFD in chemical and catalytic reaction engineering. Some of the works like Higler et al [4],Gulik[5] and Calis et al [6], deal with the hydrodynamics and mass transfer analysis in different structural catalytic packing using CFD technique.

Tertiary Butyl Alcohol (TBA) is one of the important octane enhancers in gasoline pool. More than 0.4 million ton/yr of TBA are consumed as a solvent, chemical intermediate, paint remover and high-octane gasoline additive [7,8]. Commercially it is produced by the acid-catalyzed hydration of Isobutylene. The reaction occurs in the liquid phase in the presence of 50-60% H_2SO_4 at mild temperature, the yield is approximately 95% [9]. The catalytic distillation is an integration of reaction and separation in a single vessel. Some chemicals are presently investigated on bench scale by using catalytic distillation technique [1,10,11]. One of the chemical TBA has recently been explored by Zhang et al[12] on counter current fixed bed reactor (CCFBR) configuration, which is loaded with Bales type packing. This paper study the aerodynamics of catalytic bales type packing using CFD for pressure drop simulation. Tomasz empirical correlation for dry Bales pressure drop is used for determination of FLUENT porous models coefficients and the results obtained by these correlations are compared with experimental results. The novelty of this work is the use of ANSYS Fluent software for CFD pressure drop simulation, study of internal effects of TBA reactor, and comparison of CFD results with Calis et al [6] experimental data of TBA pilot plant.

II. ANALYSIS OF FLOW DYNAMICS OF CATALYTIC PACKING BY CFD

The CFD simulations show a good output and understanding for the flow dynamics and mass transfer of following catalytic packings' used for catalytic distillation. Van Baten et al [13] obtained detailed information of liquid velocity distributions, hold-up distributions, and dispersion which is important for logical design of catalytic distillation columns.

Kloker et al [14] calculated the dry pressure drop as a function of the gas load, which is a prerequisite for the two-phase flow simulation. The simulation is performed on laminar regime. The porosity effect is represented by Ergun parameters. The CFD results are validated with the Suzlerchemtech experimental data.

2.1 Catalytic Bales type packing

The catalytic bales (CB) are extensively used as industrial packing mainly for heterogeneous processes [1,15]. The characteristics of CB packing highly depend on the flow configuration, catalyst amount loaded in the bales, column diameter and particle size [1,16,17]. The packing consists of steel mesh and glass fiber cloth, which is wrapped in the form of bales. These bales are sewn shut after catalyst beads are loaded. The resulting belt is rolled with alternating layers of steel mesh to form a cylinder of catalyst bales as shown in figure 1.

Figure 1. Bales Type Catalytic Packing

2.2 Tomasz pressure drop correlation for dry Bales packing

Tomasz empirical pressure drops for dry Bales packing is calculated on bench scale reactor used for synthesis of TBA [15]. The correlation is based on gas superficial velocity versus pressure drop, which is subsequently fitted using power law approximation with and R^2 value of 0.9881.

$\Delta P/L = 53.8836U_G^{1.707}$ (1)

WhereΔP is pressure in Kpa, L is length of Bales in meter and U_G is gas superficial velocity in m/sec. In order to optimize the variables in experimental pilot plant vessel such as gas superficial velocity, pressure drop, and liquid hold up, one should know the vessel internals' (here wall wiper) effect during simultaneous reaction and distillation. There is limited CFD literature available on the flow dynamics and mass transfer investigation of Bales type catalytic packing. Akbarnejad et al [18] modified the well-known Eckert diagrams for prediction of pressure drop in catalytic distillation columns loaded with bales and validated their model with data obtained in a pilot scale column. The limitation of their model with data obtained in a pilot scale column is that it does not predict liquid hold-up, which is an important parameter for columns. Caetano et al [17] investigated the pressure drop and liquid holdup at loading and flooding points. They developed generalized model for pressure drop and liquid holdup which is based on the model for packed distillation column of Stichlmair et al [19]. Subawalla et al [20] conducted a detailed two-phase flow dynamics and mass transfer studies on 2.1 inch diameter column. They developed a model that calculates pressure drop, capacity, and HETP for catalytic distillation packing as function of parameters such as surface area and void fraction.

III. COMPUTATIONAL FLUID DYNAMICS (CFD)

In-situ internal effects cannot be predicted physically, hence CFD is the numerical tool of predicting fluid flow, heat transfer, mass transfer, chemical reactions, and related problems by solving the sets of mathematical equations. CFD gives the detailed internal information, which is not possible, experimentally [21]. Most recently CFD been employed for the investigation of reactive distillation hardware [21,22]. The following conservation equations are used to solve CFD simulation for pressure drop and residence time distribution. The details of equations that CFD solve is given in section IV. In this paper mapping of 2D model similar to experimental reactive distillation column is presented.

The continuity equation is a declaration of conservation of mass [23].For 2D axisymmetric geometries, the continuity equation is given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v x)\frac{\partial}{\partial r}(\rho v r) + \frac{\rho v r}{r} = Sm (2)$$

Where x is the axial coordinate, r is the radial coordinate, v_x is the axial velocity, and vr is theradial velocity. The source Sm is the mass added to the continuous phase from the dispersed second phase (e.g due to vaporization of liquid droplets) and any user defined source.The vx, and vr are the axial compact way to write equation by use of Einstein notation [22].

$$\frac{\rho \partial U_i}{\partial x_i} = 0 \quad (3)$$

The momentum equation is the declaration of conservation of momentum in each of the three component directions. The three momentum equations are collectively called the Navier-stokes equation [23].

$$\frac{\partial}{\partial t}(\rho U) + \frac{\partial}{\partial xj}\left(\rho U_i U_j\right) = \frac{-\partial \rho}{\partial x} i + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2\partial Uk}{3\partial_{xk}} S_{ij}\right)\right] + \rho g_i + F_i \qquad (4)$$

The term on the left hand is convection, and on the right hand side is the pressure gradient, the source terms, the divergence of the stress tensor (which is responsible for the diffusion momentum) and the gravitational force and another generalized term respectively.

IV. METHODS AND PROCEDURE

A commercial CFD software package FLUENT 6.2 [24] was employed to predict Bales type packing aerodynamics in pilot scale reactor. FLUENT is the most widely used CFD program for modeling engineering fluid flows due to its robustness, accuracy and user friendliness. For modeling with FLUENT the three steps followed were: Pre-processing, Solver execution, and Post processing.
Pre-processinginclude Computer Aided Design (CAD) of the model, grid generation of the model, and assigning boundary conditions.

Solver execution

The operations carried out in solver execution were: Import and scale mesh file, select physical models, define material properties, prescribe operating conditions, prescribe boundary conditions, provide initial solution, set up convergence monitors, and compute and monitor solution.
Post processing includes feedback in solver and engineering analysis.

4.1 Modeling assumptions

The simulation was carried out with the following assumptions.

1. The case is two-dimensional
2. Only particle influence (Bales porosity) is considered rather than geometrical features like shape and material.
3. The gas is in turbulent flow and its distribution is uniform in the reactor.
4. Porous zone is homogenous and isotropic.
5. Flow is steady and isothermal.

4.2 Fluent modeling description

Domain consists of fifteen wall vipers, which are across 500 mm porous zone. The height of the vessel is 640 mm as shown in figure 2. To avoid higher computational efforts and memory limitation 2D domain are modeled and meshed with highly refined structural meshing scheme. Thesummary of meshing properties is shown in table 1. In order to check grid independence of solution, simulation was run on different grid size and finally 2.5 grid cell was selected.

The grid scheme, number of cells, number of nodes and size of cells were quadrilateral/mapping, 4146, 4446, and 2.5 respectively. Similarly a single CB is assumed instead of five bales with same number of wall wipers which are similar in actual model [15]. The reason for gas outlet was to avoid back flow of gas. The back flow pressure extends the convergence time of simulation [24]. The Gambit boundary and continuum types' specification shown in table 2 was assigned before domain export as a meshed file.

Length of column	640 mm
Length of porous zone	500 mm
Diameter of column	45 mm
Wall viper distance	33.33 mm
Viper dimension	6 x 2 mm
Outlet dimension	60 mm

Table 1. Dimensions of computational domain

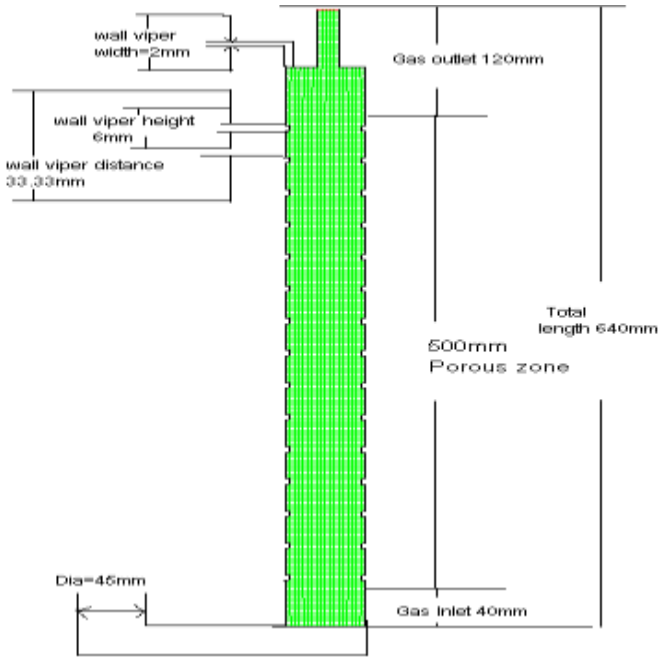

Figure 2. Computational Domain and Grid.

Gambit	Real	Type
Inflow	Gas inlet	Velocity Inlet
Outflow	Gas outlet	OUTFLOW
Fluid	Porous medium	Continuum

Table 2. Boundary types assigned in Gambit

4.3 Feed distributor

The feed gas distributor used in experimental setup was "frit" followed by small number of glass tubes, used to keep a distance between Bales and frit and distributed the gas uniformly in the column. The distance between gas frit and Bales type packing is approximately 40 mm. In computational domain similar parameters are acquired except modeling glass tubes, which was unavoidable because of complicated geometry. However glass tubes effect was negligible on flow dynamics.

4.4 Solver Execution

In order to model the fluid flow problems in FLUENT, first Fluent needs to be opened with 2ddp (two-dimensional double precision) for two-dimensional cases. The grid then needs to be inserted and checked. After the grid in place, a number of options can be defined to customize the problem to the users need. These include models, material, operating conditions, boundary conditions, and user defined scalars among others.

V. DRY PRESSURE DROP MODELING PROCEDURE

In pressure drop simulation only macroscopic effects are considered, so there is no need to perform unsteady state simulation. Similarly superficial velocity is checked because porous medium is assumed isotropic and experimental velocity is based on hydraulic diameter. The steps used for dry pressure modeling are:

Solver	Segregated
Velocity formulation	Absolute
Formulation	Implicit
Space	2D
Time	Steady
Porous formulation	Superficial velocity

The model constants are presented in table 3.

Cb1	0.1355
Cb2	0.622
CV1	7.1
CW2	0.3
CW3	2
Prandtl number	0.667

Table 3.k-ε model constant

5.1 Model Variables and boundary conditions

The model variables are dependent on Reynold numbers. The following equations are used for calculations. The turbulence intensity was estimated by the equation (5)

$$I = 0.16(Re)^{-1/8} \quad (5)$$

The turbulence kinetic energy, K was estimated by using the equation (6) below:

$$K = \frac{3}{2}(VavgI)^2 \quad (6)$$

The turbulence dissipation rate, ε was estimated by using the equation (7) below:

$$\varepsilon = \frac{C\mu^{3/4}k^{3/2}}{\ell} \quad (7)$$

Where $\ell = 0.07L$; L = Hydraulic diameter = 0.045 meter; and
$C\mu = Empiricalconstant = 0.09$

The k- ε model variables for various Reynold numbers are given in the table 4. The material type is nitrogen and its properties are listed in the table 5. The operating conditions are shown in table 6. The following boundary conditions for porous media were set up.

1. The porous zone consists of catalyst and the material flowing through the porous media is nitrogen.
2. The viscous resistance coefficients 1/α and inertial resistance C_2 is calculated using polynomial model.
3. The C_0 and C_1 are calculated using power law approximation instead of resistance coefficients and flow direction.
4. All parameters 1/α, C_2, C_1, C_0 and direction vectors are specified for combination of polynomial and power law approximation models.
5. The porosity was set to 1 as a default value.

The porous medium models coefficients calculated are summarized in the table 7. The parameters (α and C) of the media experimental pressure drop are a function of superficial velocity. The experimental pressure drop P versus superficial velocity V is shown in table 8. The use of power law model provides a better fit to Tomasz experimental data shown in the figure 3. The calculated coefficientsC_0 andC_1 atR^2 value of 1 are 26953 and 1.7077 respectively. The another advantage of using power law model is that it requires one set of coefficients [24], so the results can be analyzed by manipulating C_0 andC_1. The value of 1/α and C_2 for polynomial modelis obtained from the graph presented in figure4. This figure shows the coefficients obtained from polynomial with R^2 value of 0.9995. The gas inlet velocities used in pressure drop simulations are summarized in the table 9, which also serve as gas inlet boundary conditions. For velocity inlet the following settings were chosen.

1. The magnitude, normal to boundary was specified in velocity specification, and the velocity magnitude was set from the data of the table 8.
2. The reference frame was absolute.
3. The turbulence kinetic energy and the turbulence dissipation rate were specified from the data of the table 4.

In order to avoid reverse flow problem and minimize convergence difficulties the following pressure outlet boundary conditions were selected.

1. The gauge pressure (pascal) was set to zero.
2. The back flow turbulence kinetic energy and turbulence dissipation rate was set to 1.
3. Normal to boundary was selected in back flow direction specification method.

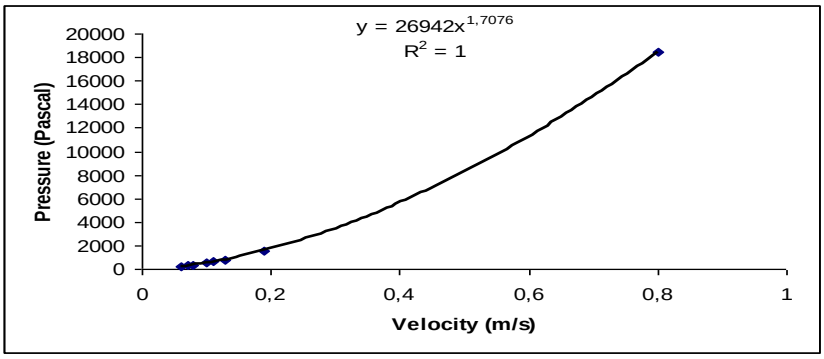

Figure 3. Power approximation fitting for experimental pressure drop data.

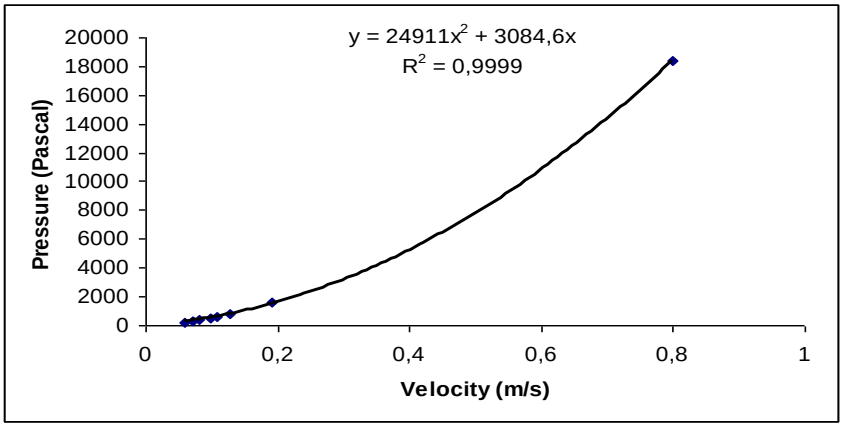

Figure 4. Coefficients obtained from polynomial expression.

Reynolds Numbers	Turbulence Intensity	Turbulence kinetic energy(m**2**/s**2**)	Turbulence Dissipation rate m**2**/s**3**
188	0.083	3.72e-5	1.18e-5
218	0.081	4.80e-5	1.73e-5
248	0.08	6.14e-5	2.50e-5
307	0.078	8.9e-5	4.40e-5
337	0.077	1.05e-4	5.60e-5
396	0.075	1.41e-4	8.63e-5
586	0.072	2.8e-4	2.37e-4
1542	0.063	1.4e-3	2.66e-3
2468	0.060	3.4e-3	0.010

Table 4.k-ε model variables for above Reynolds numbers

Density kg/m3	1.138
Cp j/kg-k	1040.67
Thermal conductivity w/mk	0.0242
Viscosity kg/m-sec	1.66e-5

Table 5. Material properties

Parameters	**Specification**
Operating pressure (Pascal)	101325
Gravity	- 9.81m/sec2 (y direction)
Operating density (kg/m3)	1.225

Table 6. Operating parameters

a	24000
b	3935
C (1/m)	42179
1/α (1/m2)	237048193
C0	26953
C1	1.7077

Table 7. Calculated coefficients for porous boundary conditions

Gas superficial velocity (m/sec)	Experimental Pressure drop (pascal)
0.06	221
0.07	287
0.08	361
0.099	519
0.109	612
0.128	806
0.19	1582
0.5	8252
0.8	18400

Table 8. Experimental Pressure drop as a function of gas superficial velocity

Reynolds Numbers	Gas superficial velocity (m/sec)
188	0.06
218	0.07
248	0.08
307	0.099
337	0.109
396	0.128
586	0.19
1542	0.5
2468	0.8

Table 9. Gas superficial velocity inlet boundary conditions

VI. RESULTS AND DISCUSSION

The data was validated, the behavior (contours/vectors) of fluid across catalyst packing was analyzed, and the results are discussed here. For pressure drop simulation the three techniques that are power law model, polynomial model and combination of the two were used. In power law model, the measured CFD pressure drop is lower than the experimental pressure drop. It can be observed that at lower velocity range, the curve is quite satisfactory but as the velocity range goes up, the difference increases significantly. The comparison between experimental and predicted CFD pressure drop is presented in the figure 5. In order to achieve the same experimental curve, the CFD simulation was rerun after the modifying the value of coefficient C_0 but keeping the C_1 same. The modified value of C_0 was obtained by dividing the experimental pressure drop with CFD pressure drop as shown in table 10. The average of the factor obtained is 2.3745. After multiplying this average factor with Tomasz, the dry bales empirical correlation equation (1) becomes:

$\Delta P/L = 2.3745x\ 53.8836\ U_G^{1.707} \rightarrow 127.94\ U_G^{1.707}$

The simulation on modified C_0 was rerun; the results obtained (shown in figure 6) were the same as experimental results. The three reasons for modifying the Tomasz empirical correlation were that i) both Tomasz's empirical correlation and the CFD model are derived from the power law relationship, ii) relatively easy to compute since they require only one set of coefficients, and iii) to attain the actual pressure drop, which was the primary objective of this research study.

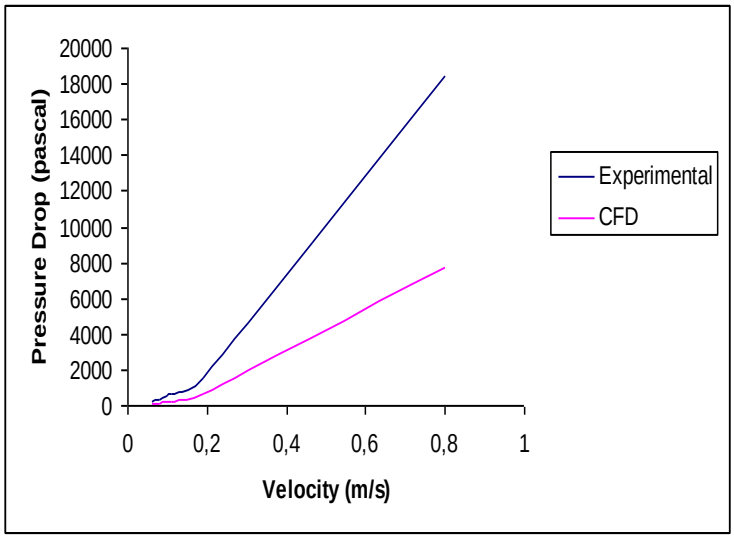

Figure 5. Comparison between experimental and predicted CFD pressure drop.

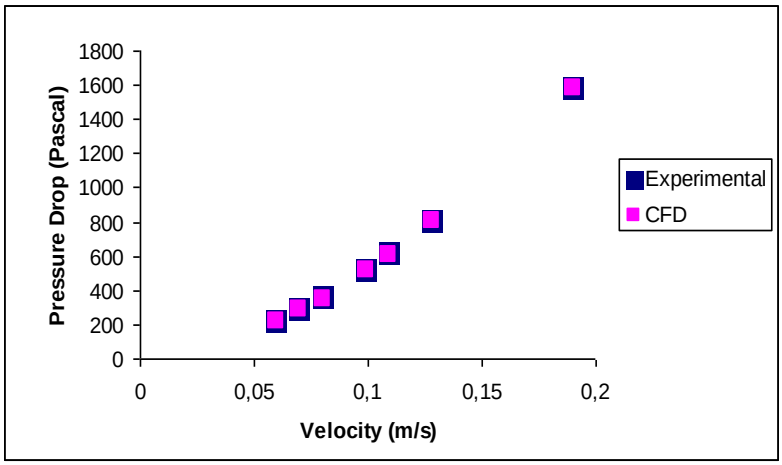

Figure 6. CFD results on modifying Value of Coefficient C_0.

Experimental Pressure drop	CFD pressure Drop	Factor
221	93	2.3763
361	152	2.3750
519	218	2.3807
612	260	2.3740
806	340	2.3703
18407	7780	2.3672

Table 10. Factors used for modifying C_0

The pressure drop computed by polynomial model shows similar behavior as the power law model, as shown in figure 7. However, at higher velocity range, the polynomial model diverges slightly from the power law model. If the data is extrapolated, this difference is further increased. In both models the reason for the higher deviation of CFD results from experimental pressure drop is mainly due to the poor prediction of the turbulent contribution. The velocity range used in the simulation was in transition region, whereas Fluent computed by taking into consideration only the approximated effects of the turbulence in the porous medium [24].

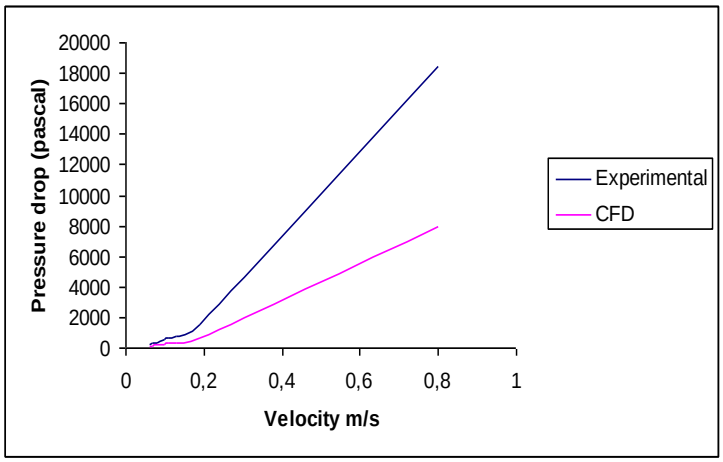

Figure 7. Experimental versus CFD Pressure drop.

The combination of the power law and the polynomial model clearly indicate an excellent agreement with experimental results. It can also be noticed that k-ε model shows a good correlation with Ergun equation. The figure 8 shows the contour plot and the velocity vector obtained from combined model at v = 0.06 and 0.19 m/s. The comparison of experimental results with CFD predicted results for pilot scale column is shown in figure 9.

The average deviation of power law and polynomial model from the experimental results are 57% and 50% respectively. It can also be seen that the agreement between the experimental and the simulated pressure

drop using combination of power law and polynomial model is better with and an average deviation of 13%, which is certainly acceptable in the design [25].

The CFD simulations and results indicate that the CFD model is not only able to predict an integral performance characteristic like the pressure drop, but also local velocities. Consequently it is anticipated that CFD simulation of catalytic Bales aerodynamics can be of significant help in obtaining a detailed understanding of the physical phenomena that take place in a bench scale column with catalytic bales packing.

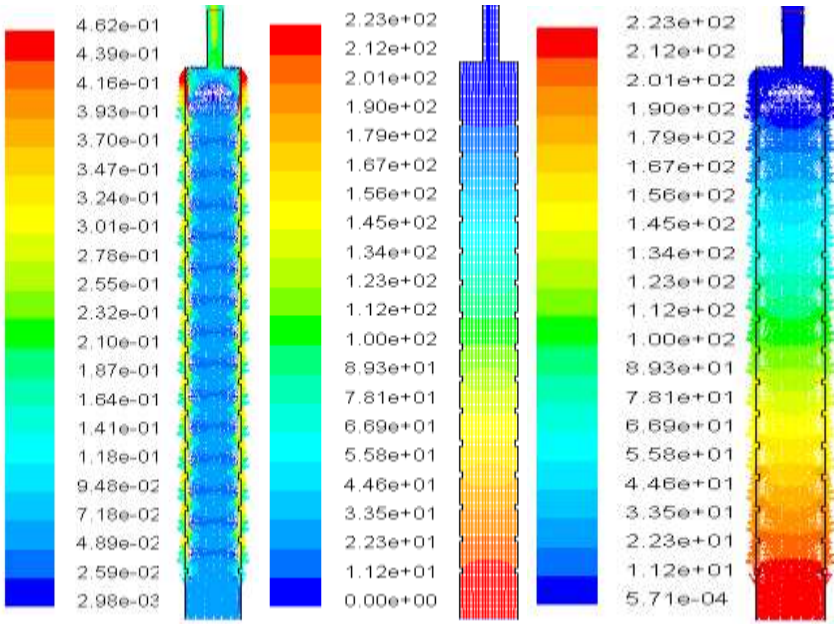

Figure 8. Velocity vector and contour plot profile using combined model.

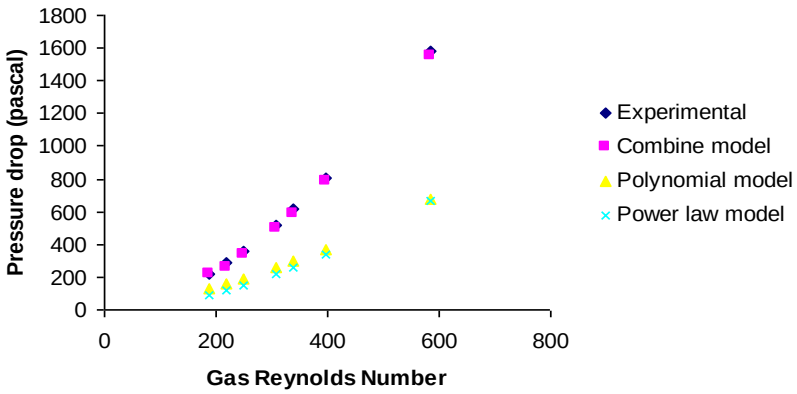

Figure 9. Comparison of pressure drop Vs Reynolds numbers of all three models.

VII. CONCLUSION

This study shows that a commercial CFD (FLUENT) code can be used to predict the aerodynamics of a catalytic Bale packing in terms of pressure drop. It was found that the CFD simulations for pressure drop over a wide range of relevant Reynolds numbers, predicted by combination of power law and polynomial models show a good agreement with the experimental pressure drop data.

The CFD simulation without wall wipers show uniform velocity profile indicative of axial velocity in the column. The CFD model revealed that due to wall wipers, the gas radial velocity increases significantly and there is a reduction in the gas axial velocity, which reduces the pressure drop. In addition, the simulations without the wall wipers show the actual pressure drop solely due to the catalytic bales and thus it can help to modify the Tomasz empirical correlation for dry Bales.

It is concluded that the advantages of the wall wipers' are two fold; firstly they improve the gas aerodynamics by lowering the pressure drop and increases mixing and secondly they minimize the mal-distribution or by-passing in the column.

The CFD simulation study presents detailed aerodynamics of bench scale reactor plugged with catalytic Bales, and proves that CFD is an efficient diagnostic tool for such type of investigation.

Nomenclature

C Concentration of tracer (-)
Co Empirical coefficient (pa/m)
C_1 Empirical coefficient (-)
C_2 Inertial resistance coefficients, (1/m)
ε Turbulence dissipation rate
I Turbulence intensity
k Turbulent kinetic energy, m^2/s^2
L length of bales, m
P pressure, Pascal
Re_g Gas Reynolds number
R^2 Coefficient of determination
U Gas superficial velocity, m/s

Greek- letter

α Permeability, m^2
ε Porosity,(-)
μ Viscosity, kg/ms

Abbreviations

CAD Computer Aided Design
CB Catalytic Bales
CCFBR Counter Current Fixed Bed Reactor
CD Catalytic distillation
CFD Computational Fluid Dynamics
FLUENTA modeling software
HETP Height Equivalent to a Theoretical Plate
TBATertiary Butyl Alcohol

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