Recent Developments in Year 2000s in the Modelling of Turbulence Transport in Catalysis

Oyegoke Toyese,
Laboratoire de Chimie, ENS, l'Universite de Lyon, Lyon, France
Department of Chemical Engineering, Ahmadu Bello University Zaria, Nigeria
Toyese.oyegoke@ens-lyon.fr, OyegokeToyese@gmail.com
and
Adamu Yusuf,
Department of Chemical Engineering, Ahmadu Bello University Zaria, Nigeria
Edomwonyi-Otu C. Lawrence,
Department of Chemical Engineering, Ahmadu Bello University Zaria, Nigeria.
Department of Chemical and Petroleum Engineering, Delta State University, Nigeria
Akanji N. Abiodun
Department of Chemical Engineering, Ahmadu Bello University Zaria, Nigeria.
Department of Chemical Engineering Technology, Federal Polytechnic Bida, Nigeria

Abstract: The turbulent nature of catalytic reactions has been well reported. For some reactions, the higher the rate of turbulence, the faster the reaction process. This paper focus on the review of various research works where turbulence models were employed in promoting and advancing study and knowledge of catalysis or catalytic reaction systems (such as fixed bed reactor, trickle bed reactor, combustor, among others) or processes in the twentieth centuries. It also draws attention to several fluid computational dynamics package employed in the simulation and different contributions that have been made in advancing research in the field of catalysis via turbulence modeling. The essence of these is to enhance effective and efficient reactant access to the active sites of the catalyst. This study, however, shows that models such as k–e and RSM turbulence models are better suited for predicting or studying turbulence behavior in a catalytic reaction. It was realized that apart from selecting the turbulence model, appropriate selection of the kinetic model plays a significant role in promoting accurate prediction when carrying out simulations. However, this study was able to identify that only a few research works have given attention to the right and appropriate use or selection of a kinetic model for catalytic reaction systems.

Keywords: Simulation, Transport Phenomena, Kinetic Model, Chemical Reactors, Turbulence.

التطورات الأخيرة في العام ٢٠٠٠ في نمذجة النقل المضطرب بالتحفيز

الملخص: تم الإبلاغ جيدًا عن الطبيعة المضطربة للتفاعلات التحفيزية. بالنسبة لبعض التفاعلات، كلما زاد معدل الاضطراب، زادت سرعة عملية التفاعل. تركز هذه الورقة على مراجعة الأعمال البحثية المختلفة حيث تم استخدام نماذج الاضطراب في تعزيز وتطوير الدراسة والمعرفة بأنظمة الحفز أو التفاعل التحفيزي (مثل مفاعل السرير الثابت، مفاعل السرير المقطر، جهاز الاحتراق، من بين أمور أخرى) أو العمليات في القرن العشرين. كما يلفت الانتباه إلى العديد من حزم ديناميكيات حساب السوائل المستخدمة في المحاكاة والمساهمات المختلفة التي تم إجراؤها في تطوير البحث في مجال التحفيز عبر نمذجة الاضطراب. يتمثل جوهر هذه العناصر في تعزيز الوصول الفعال والكفؤ للمتفاعلات إلى المواقع النشطة للمحفز. ومع ذلك، تُظهر هذه الدراسة أن نماذج مثل نماذج الاضطراب k-e وRSM هي أكثر ملاءمة للتنبؤ أو دراسة سلوك الاضطراب في تفاعل تحفيزي. تم إدراك أنه بصرف النظر عن اختيار نموذج الاضطراب، يلعب الاختيار المناسب للنموذج الحركي دورًا مهمًا في تعزيز التنبؤ الدقيق عند إجراء عمليات المحاكاة. ومع ذلك، تمكنت هذه الدراسة من تحديد عدد قليل فقط من الأعمال البحثية التي قد أعطت اهتمامًا للاستخدام الصحيح والمناسب أو اختيار نموذج حركي لأنظمة التفاعل التحفيزي.

1. Introduction

Turbulence flow is a type of flow regime in fluid dynamics characterized by flow velocity and disordered change in pressure [1]. This phenomenon is often observed in routine processes like billowing storm clouds, fast-flowing river, surf, or smoke from its different bases. Turbulent Fluid flows occur in the natural and engineered system and other related applications [2-4]. It is commonly driven by substantial kinetic energy within the flowing fluid in excess of the prevailing viscous absorbing effect of the flows. This shows that turbulent effects are more challenging to create in high viscosity fluids than in low viscous fluids. The prediction of turbulence is often quantified by a dimensionless physical quantity (or constant) known as Reynolds number from inception, which signifies the proportion of kinetic energy to the amount of the viscous damping present in a flow. However, due to the lengthy resistant detailed physical analysis in turbulence coupled with the interactions holding within, which created a very complicated situation. Richard Feynman has identified that turbulence as a crucial unresolved challenge in the classical physics field [5].

Turbulence is often identified to be irregularity or randomization, which indicates that turbulence problems can be solved statistically instead of solving the problem deterministically. Also, it is known to be chaotic and disorganized. However, not all disorganized flows are turbulent [6]. Turbulence flows are also characterized by diffusivity (which tends to increase the homogeneity of the mixing components in the fluid), rotationality, and dissipation. The turbulent flows which are dissipative make it necessary to make provision for a constant generation of energy supply to sustain it like in the case of hydro-power supply. The dissipation of turbulence does hold when a substantial kinetic energy present in the fluid gets converted into internal energy employing viscous shear stress [7].

This paper focus on the review of different research works where turbulence models are employed in promoting and advancing studies and knowledge of catalysis or catalytic reaction systems or processes in the twentieth century.

2. Catalysis

Catalysis, a field of study that deals with reaction systems and its ways of speeding up the number of chemical species interaction and conversion due to the influence of a catalyst. In this process, the catalyst is not consumed but can be repeatedly used. During these chemical reaction processes, catalysts are not used up or consumed by the primary processes but can be deactivated, prevented, or destroyed by secondary processes (that is, side reactions). For instance, side reactions like dissolution, coking, scission, or sublimation, on a heterogeneous

catalyst [8-11]. In most cases, only a small quantity of catalysts is required in principle. In general, the catalyst influences the reactions to hold faster due to lower energy requirements due to the low activation energy [11, 12].

Studies have revealed that catalyzed reactions display lower activation energies than the corresponding analyzed un-catalyzed reactions, yielding a higher rate of chemical reaction, at the same thermal conductivity and the same reaction density. However, the details of the mechanics for catalysis are intricate. Catalysts fundamentally influence the environment of the reaction and support the reagents to have the positive bonds polarized, e.g., Acid catalysts used in the formation of naturally occurring intermediates (specific), or the reactions of carbonyl compounds, like osmate esters present in the dehydroxylation of osmium tetroxide-alkynes. Physically, most catalytic reactions are often chemical reactions; The rate of these chemical reactions often depends on the reaction contact frequency with the catalyst surface when overcoming the energy complex of the rate-determining step (RDS) in its reaction path [13]. Generally, the catalyst's participation is at a slower pace, and the rates are controlled via the amount and activity of the catalyst. The diffusion rate to the reaction surface and the diffusion behavior of the products from the surface can be easily determined in heterogeneous catalysis. ZSM-5 is an excellent example of a solid catalyst [14].

Catalysts may be categorized into either heterogeneous (otherwise known as a solid catalyst) or homogeneous catalysts, and other bio-catalysts, otherwise known as enzymes, are often considered a third category. Several works in diverse areas of research have employed different catalysts to enhance their reaction processes or steps. Some of these works that used homogeneous catalysts are the work of Vicente et al. [15] in biodiesel production where nearly 100 wt% yield was obtained for the use of methoxide catalyst while the review of Johnson et al. [16] report indicates the use of the homogenous catalyst for the dehydrogenation of alcohol for the production of hydrogen will only be feasible low molecular weight alcohols (MWA) like methanol, ethanol, and isopropanol, unlike larger MWA.

Whereas those that employ the use of heterogeneous catalyst includes Helwani et al. [17] review unveiled that the use of a solid catalyst better enhances the triglycerides transesterification process than enzymes; Oyegoke et al. [18] in the dehydrogenation of propane into propylene employed the use of solid catalyst where the studies indicate that the Cr site was the most active and reactive site the promote the hydrogen abstraction from the feed. Further, Zhao et al. [19] in solar water oxidation showed a high activity towards the reaction, while Morales-Delarosa et al. [20] in the cellulose hydrolysis into fermentable sugar,

and many others with a resulting conversion >99 % after 5 h of reaction and with 87 % glucose yield.

Biocatalysts are developed by Gao et al. [21] for the enhancement of enzymatic reaction, which results in glycerol conversion and Glycerol carbonate yield as 85.20 %, and 64.71%, respectively after 24 h. Likewise, Cubides-Roman et al. [22] employed the use of an enzyme to accelerate biodiesel production, resulting to a low optimum conversion 9.6 %, while Das et al. [23] studies indicate that the prepared nano biocatalysts appear to be potent catalysts for successful industrial applications, especially in food industries. In general, the catalyst could be some transition metals, transition metal complexes, and/or enzymes.

3. Mechanism of Catalytic Reactions

According to Matthiesen et al. [24], catalysts often interact with different reacting species in a chemical reaction to form intermediate surface species (which are often said to be unstable product) that subsequently gets transformed into the desired products and some undesired ones. The presence of theses undesired products that often get stocked on the catalyst surface has made it necessary to regenerate the catalyst by getting rid of the deposited materials' surface before recycling it. The scheme presented in equations 1 to 5 is a reaction system that is common in which C stands for the catalyst, with P as a product while A and B represent reacting species:

$$C + A \rightarrow CA \quad (1)$$

$$B + CA \rightarrow BCA \quad (2)$$

$$BCA \rightarrow CP \quad (3)$$

$$CP \rightarrow C + P \quad (4)$$

The scheme indicated that the catalyst (C) was used up by reaction 1, and it was after that released in reaction 4, so the catalyst is not always displayed in the chemical expression for the overall reaction in equation 5, indicating that catalysts are neither transformed nor destroyed [25, 26].

$$A + B \rightarrow P \quad (5)$$

The recovery of catalysts shown in the scheme indicates the only a small amount is needed to influence the speed of a chemical reaction. Sometimes, catalysts are used-up in secondary processes, not often. Catalyst is not expressed in a rate expression (or equation), e.g., if the foremost step in the displayed reaction process is taken as the one that determines the reaction rate (rate-determining step, RDS), the network of catalyst influenced reaction is then a second-order reaction with the rate given as; $v = k_{cat}[A][C]$ when RDS approximation is adopted for the rate, which indicates that it varies directly with the catalyst concentration [C]. The [C]

remains unchanged for the period of the reaction, while the catalyzed reaction is pseudo-first-order written in the form: $v = k_{obs}[A]$, where $k_{obs} = k_{cat}[C]$ (Matthiesen et al. [24]). A catalyst can influence the change in equilibrium concentration in a continuous process, but this is, however, contrary to the laws of thermodynamics [24].

4. Turbulence Models Used in Catalysis

Modeling of turbulence is the method of constructing and making use of models (in forms of mathematical expressions) for the prediction and comprehension of turbulence phenomena in engineering or scientific processes or systems. Turbulent fluid flow exhibits traits or capabilities on different scales like timescale, length-scale, and so forth, which all interact with each other [27]. In the work of Ching [28], it was identified that a common approach employed in the field of turbulence modeling is to norm the main equations of the flow rate and to zero in on large-scale and flow's laminar components.

Nevertheless, it is necessary to model the effects of the fluctuating and small scales region in turbulence [28, 27]. A further survey of the literature unveils that several turbulence transport-models such as K-epsilon (k–ε), Reynolds Stress Model (RSM), and Spalart Allmaras (*s-a*) have been employed in the simulation of computational fluid dynamics (CFD). Table 1 displayed the various CFD based research works done so far. Further reports in this section present a summary of commonly applied turbulence equations and models that have been found useful in recent reaction engineering processes, and reports of other research work where they are employed with special attention for catalysis-based studies.

4.1 k–epsilon (k–ε)

The typical model often applied in CFD is the K-epsilon (k-ε) turbulence equations, which could be used to study mean flow properties for turbulent flow situations. It is can also be known as a two-equation model that reveals the general behavior of turbulence via the use of two (2) transport models (PDEs). As reported by [28], the kinetic energy of turbulence, k, can be expressed as:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_i)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right] + 2\mu_t E_{ij}E_{ij} - \rho\varepsilon \tag{6}$$

While the dissipation [28], ε will be in the form:

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \frac{\partial(\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right] + C_{1\varepsilon}\frac{\varepsilon}{k}2\mu_t E_{ij}E_{ij} - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} \tag{7}$$

Where u_i represents velocity component in the corresponding direction, E_{ij} represents the component of the rate of deformation, μ_t represents eddy viscosity given as:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}$$

The models also consist of some adjustable constants such as $\sigma_k, \sigma_\varepsilon, C_{1\varepsilon}$, and $C_{2\varepsilon}$. These constant values have were obtained via numerous iterations of data fitting for a wide range of turbulent flows which were reported as $C_\mu = 0.09$, $\sigma_k = 1.00$, $\sigma_\varepsilon = 1.30$, $C_{1\varepsilon} = 1.44$, and $C_{2\varepsilon} = 1.92$ in literature.

The improved model of the mixing-length equations was identified to be the K-epsilon model, including the provision of a replacement to the algebraically prescribed turbulence and fluctuating length-scale of measurement in medium to very complex flows. Research works of Christoph et al. [29] employed the *k-e* representative equations to investigate turbulence in a combustion process, within channel flows, of the mixture of hydrogen and air over a stabilized platinum catalyst. With the use of a *k-e* model, Muhammad [30]) studied the CFD prognostication of profile displaying mass fraction of gasoline and gas oil in a fluid catalytic cracking (FCC) riser main. Using the k-epsilon turbulence model and 4-lump model, the same author in 2013 also examined an FCC riser to predict gasoline yield.

In 2014, an analysis of the material flow within a radial flow fixed bed (FB) reactor was conducted by Dominick et al. [31]. Following this, Afshin [32] evaluated the effect of carbon tetrachloride (CCl_4) addition as propulsion to the thermal cracking reactor as a result of the coke formed in separate coil outlet temperatures (COT). Both Dominick et al. [31] and Afshin [32] employed *k-ε* models.

This model is simple, affordable, and considerably accurate for a wide variety of flow that lacks separation. Literature indicates that this model often failed to give an accurate prediction for the onset and the flow separation under the adverse pressure gradient [1, 28, 33].

4.2 Menter's Shear Stress Transport (SST)

SST (Menter's shear stress transport model) turbulence model is one of the most robust two-equation eddy-viscosity turbulence models often used in CFD [33]. The model combines both the k-omega turbulence model and the K-epsilon turbulence model, such that the k-omega model is employed in the boundary layer inner region and switches to the k-epsilon model in the free shear flow system.

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho u_j k)}{\partial x_j}=P-\beta^*\rho\omega k+\frac{\partial}{\partial x_j}\left[\left(\mu+\sigma_k\mu_t\right)\frac{\partial k}{\partial x_j}\right] \tag{8}$$

$$\frac{\partial(\rho\omega)}{\partial t}+\frac{\partial(\rho u_j \omega)}{\partial x_j}=\frac{\gamma}{\nu_t}P-\beta\rho\omega^2+\frac{\partial}{\partial x_j}\left[\left(\mu+\sigma_\omega\mu_t\right)\frac{\partial\omega}{\partial x_j}\right]+2(1-F_1)\frac{\rho\sigma_{\omega 2}}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial\omega}{\partial x_j}$$

(9)

Here, $P=\tau_{ij}\frac{\partial u_i}{\partial x_j}$ $\tau_{ij}=\mu_t\left(2S_{ij}-\frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right)-\frac{2}{3}\rho k\delta_{ij}$,

$S_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)$, $\mu_t=\frac{\rho a_1 k}{\max(a_1\omega,\Omega F_2)}$,

$\phi=F_1\phi_1+(1-F_1)\phi_2$, $F_1=\tanh\left(\arg_1^4\right)$, $\arg_1=\min\left[\max\left(\frac{\sqrt{k}}{\beta^*\omega d},\frac{500\nu}{d^2\omega}\right),\frac{4\rho\sigma_{\omega 2}k}{\mathrm{CD}_{k\omega}d^2}\right]$,

$\mathrm{CD}_{k\omega}=\max\left(2\rho\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial\omega}{\partial x_j},10^{-20}\right)$, $F_2=\tanh\left(\arg_2^2\right)$, $\arg_2=\max\left(2\frac{\sqrt{k}}{\beta^*\omega d},\frac{500\nu}{d^2\omega}\right)$

The constants $\sigma_{k1}=0.85,\sigma_{w1}=0.65,\beta_1=0.075$ for the k-w closure, the constants for the k-e closure, where $\sigma_{k2}=1.00,\sigma_{w2}=0.856,\beta_2=0.0828$, while $\beta^*=0.09,a_1=0.31$ were the SST's closure constants. The boundary/wall/far-field conditions are given as follows:

$$\frac{U_\infty}{L}<w_{\text{farfield}}<10\frac{U_\infty}{L},\frac{10^{-5}U_\infty^2}{Re_L}<k_{\text{farfield}}<\frac{0.1U_\infty^2}{Re_L},\ \omega_{wall}=10\frac{6\nu}{\beta_1(\Delta d_1)^2},k_{wall}=0$$

The SST model has reported being highly accurate for the predictions of the onset and the amount of flow separation under adverse pressure gradients via the introduction of transport effects into the formulation of the eddy-viscosity. Also, despite being a blend of k-ω and k-ε, that is a k-ω model near the wall and transitions to a k-ε model away from the wall. The model has been reported to be relatively insensitive to the free stream value of ω. [1, 28, 33]

4.3 k–omega (k–ω)

In CFD, the k–omega (*k–ω*) turbulence representative equation is a popular two-equation model, which is often employed as a solution for the Reynolds-averaged Navier–Stokes (RANS) equations [34]. The representative equation is designed to unveil turbulence profiles via the use of 2-partial derivative equations for 2-variable quantity k and ω, where k is the upheaval kinetic energy. In contrast, ω is the specific dissipation rate of the kinetic energy (k) of turbulence to obtain internal thermal energy.

Mathematically, the eddy viscosity ν_T, as required in the RANS equations, is expressed as $\nu_T = k/\omega$, and the development of k and ω is mathematically represented [28] in the form:

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho u_j k)}{\partial x_j}=\rho P-\beta^*\rho\omega k+\frac{\partial}{\partial x_j}\left[\left(\mu+\sigma_k\frac{\rho k}{\omega}\right)\frac{\partial k}{\partial x_j}\right],\qquad \text{with } P=\tau_{ij}\frac{\partial u_i}{\partial x_j}, \tag{10}$$

$$\frac{\partial(\rho\omega)}{\partial t}+\frac{\partial(\rho u_j \omega)}{\partial x_j}=\frac{\alpha\omega}{k}P-\beta\rho\omega^2+\frac{\partial}{\partial x_j}\left[\left(\mu+\sigma_\omega\frac{\rho k}{\omega}\right)\frac{\partial\omega}{\partial x_j}\right]+\frac{\rho\sigma_d}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial\omega}{\partial x_j} \tag{11}$$

Where k is the turbulence kinetic energy, ω is the specific rate of dissipation (of the turbulence kinetic energy k into internal thermal energy), ν_T is kinematic eddy viscosity. The coefficients were reported as $\alpha=5/9$, $\beta=3/40$, $\beta^*=9/100$, $\sigma=1/2$, $\sigma^*=1/2$, and $\varepsilon=\beta^*\omega k$.

This model has been reported to have shown an advantageous feature for integrating through a viscous sub-layer and inflows with adverse pressure gradients, being a two-equation model, which have adequate representation for both scales independently. The literature further indicates that the k-ω models are more accurate and numerically stable in the near-wall region [1, 28, 34].

4.4 Reynolds Stress Model (RSM)

The RSM, also known as the second-moment closure representative equations, is the most complete of the classical turbulence modeling approach. It is mathematically expressed as follows:

$$\frac{DR_{ij}}{Dt}=D_{ij}+P_{ij}+\Pi_{ij}+\Omega_{ij}-\varepsilon_{ij} \tag{12}$$

Where R_{ij} is $\langle u_i' u_j' \rangle = -\tau_{ij}/\rho$, D is diffusion-controlled transport of R_{ij}, P is R_{ij} production speed, Π is R_{ij} transport resulting from interactions of turbulent pressure-strain, Ω is R_{ij} transport resulting from rotation, ε is dissipation speed of R_{ij}.

The eddy-viscosity representative equations are well known and include the *k–e* (k–epsilon) and the *k–ω* (k–omega) equations, which have weaknesses in sophisticated flows applicable in engineering. The findings were a result of the use of hypothesizing with the eddy-viscosity equations in their articulation. For example, in a flow with high levels of anisotropy, separation of flows, areas of recirculating flow, rotational-effects flows, or the significant streamline curvature, these models performed very poorly [35]. In these sets of flows, RSM offers superior prediction quality [36]. Closures based on Eddy viscosity are not able to explain the reversal to the isotropy of turbulence, which is noticed in the decaying of turbulent flows [37]. Models based on Eddy viscosity are not able to cannot produce replicas of the properties of a turbulent

flow in the fast-paced deformation limit, where a flexible system indicates the behavior of a turbulence flow [38].

Reynolds stress models have been reported to have displayed better accuracy significantly when compared with turbulence models although, it is expensive (that is, significantly slower to solve its set of equations), and it requires a good initial guess. Generally, suffer from numerical stability issues due to the complexity of the modeled terms, which was one of the key reasons why the models are not regularly employed in a large-scale problem [33, 34].

Table 1: Different applications of turbulence models in catalysis

Author	Research Works	Turbulence Model (s) Used
Christoph et al. [29]	An experimental and numerical study of turbulent in a channel flow combustion (CST) of air-hydrogen mixtures over stabilized platinum catalysts.	Closure of Turbulence was attained via Low Reynold *k-ε* models.
Rodrigo and Rosa [40]	Modeling of turbulence present in a multi-phase flow in a high-pressure trickle-bed reactor (TBR).	*S-k-ε*, *R-k-ε*, RNG and RSM models.
Binxin [41]	Examination of turbulence models for non-Newtonian fluid flow in anaerobic digesters via the use of the CFD approach.	low-Reynolds-number (LRe) k-ε, high-Reynolds-number (HRe) *k-ε, k-ω*, and the RSM.
Muhammad [30]	The prediction of gas oil and gasoline's mass fraction profiles in an FCC riser via the CFD approach.	*k-ε* model
Muhammad [43]	Using CFD to predict the yield of gasoline in an FCC riser by applying *k*-epsilon turbulence and 4-lump kinetic representative equations.	*k-ε* model
Xiaomin et al. [39]	Using CFD modeling for the study of reaction kinetics in a catalytic dehydrogenation of syngas in a fixed-bed reactor	Spalart–Allmaras *(s-a*)
Dominick et al. [31]	The flow was analyzed in a radial flow fixed bed reactor	A RANS type *k-ε* turbulence model
Zhapbasbayev et al. [42]	Modeling of turbulent flow behavior in a radial reactor with a fixed bed configuration	Reynolds motion equations and k-ε model
Afshin [32]	The addition of CCl_4 propulsion to the thermal cracking reactor as a result of the coke produced in separate coil outlet temperatures (COT) was evaluated	Standard *k-ε*, and RNG *k-ε* models.

4.5 Spalart–Allmaras (s–a)

One of the one-equation models that solve a modeled transport mathematical expression for motion-focused eddy fluctuating viscosity is the Spalart–Allmaras (*s-a*) model. The model was explicitly developed for systems that involve flows in the direction of the wall and showed that good results were obtained when boundary layers were controlled by opposing pressure gradients. Progressively, it is being accepted as essential in turbo-machinery applications.

The model is expressed as follows:

$$\frac{\partial \tilde{\nu}}{\partial t} + U_j \frac{\partial \tilde{\nu}}{\partial x_j} = P_{\tilde{\nu}} - \epsilon_{\tilde{\nu}} + \frac{\partial}{\partial x_j}\left[\frac{1}{\rho}\left(\mu + \frac{\tilde{\nu}}{\sigma_{\tilde{\nu}}}\right)\frac{\partial \tilde{\nu}}{\partial x_j}\right] \quad (13)$$

A survey of literature has indicated that this model does not accurately compute fields that exhibit separated flow, shear flow, or decaying turbulence due to the absence of a correction factor for compressibility, resulting in the model's overpredict the growth rate of high-speed shear layers. Although, the model has shown for giving good results for boundary layers and adverse pressure gradients [1, 28, 34].

Moreover, Xiaomin et al. [39] modeled the turbulence behavior of the reacting species in the use of a catalyst to remove hydrogen from syngas in a fixed-bed (FB) reactor by applying the *s-a* model to unveil some information about the reaction kinetics.

Some other research works employed several turbulence models to screen out the best model that gave the best prediction for the concern system chosen for the study. In line with this approach, Rodrigo and Rosa [40] employed the use of *k-e* and RSM models for the representation of turbulence behavior in two or more fluid flows in trickle bed reactors under high pressure. At the same time, Binxin [41] investigated the turbulence representative equations for non-Newtonian fluid flow behavior in an anaerobic digester using the *k-ε*, RSM, and *k-ω* representative equations.

Furthermore, Zhapbasbayev et al. [42] model a turbulent flow present in a radial reactor with a fixed bed using Reynolds motion equations and *k-ε* models. *S-k-ε*, *R-k-ε,* RNG, RSM, and *s-a* can be used for a fixed bed reactor to model turbulence transport in catalysis. However, the review shows that *k-e* models are commonly employed in this practice, unlike RNG, RSM, or *s-a*.

5. CFD Packages Commonly Used in the Modelling of Turbulence in Catalysis

Computational fluid dynamics with the acronym 'CFD' is a field of study in fluid mechanics that deals with the use of numerical analysis and data structures to provide solutions and analytical parameters for problems that involve fluid flow. In this area of fluid mechanics, computers are employed to execute several calculations or computations required to simulate or evaluating the interaction of gases and liquids with surfaces distinction by boundary conditions. The use of CFD analysis has made it realistic to enable quick, efficient simulation of heat transfer and fluid flow through the use of software (Solid Works). Examples of the software or packages are Gambit, FLUENT, COMSOL Multi-physics, and many others. These

applications have long been employed in the study of the turbulence flow in a catalytic system such as combustors, TBRs, bio-digesters, FCC riser reactor, fixed-bed reactors, cracking reactors, and so on as presented in the literature [29-32, 39-42].

Table 2 - Computational fluid dynamic packages commonly used in catalytic systems

Author	System Studied	Software Used
Christoph et al. [29]	Hydrogen/air mixtures in a bed of platinum in a combustor.	CHEMKIN
Rodrigo and Rosa [40]	Flow in trickle bed reactor (TRB)	Fluent 6.1 software, Gambit, PC-SIMPLE.
Binxin [41]	Studied flow in an anaerobic digester	Gambit 2.4.6 and Fluent 12.0
Muhammad [30]	FCC riser reactor (Alumina used as a catalyst)	FLUENT 6.3 was employed.
Muhammad [43]	FCC riser reactor (Alumina used as a catalyst)	FLUENT 6.3
Xiaomin *et al.* [39]	Syngas in a heterogeneous fixed-bed reactor (FBR)	FLUENT 6.3.26, SIMPLE
Dominick et al. [31]	Evaluate of radial flow behavior in a fixed bed reactor	COMSOL Multi-physics
Zhapbasbayev*et al* [42]	Flow in a duct with porous medium (or flow in a pipe with a fixed bed)	Not reported
Afshin [32]	Thermal cracking reactor	Not reported

A review of the literature shows that the FLUENT package has been the most common package employed in CFD analysis of the catalysis, turbulence modeling works like Rodrigo and Rosa [28], Binxin [41], Muhammed [30, 43], and Xiaomin et al. [39] were some of the authors that employed the use of FLUENT package for their studies. Table 2 summarizes different CFD packages commonly used in catalysis. The study of works that employed the use of CFD packages to analyze their systems is Christoph et al. [29] that CHEMKIN used for chemical kinetics and laminar transport data evaluation of hydrogen-air combustor. Moreover, Binxin [41] employed the used Gambit 2.4.6 for meshing, while Fluent 12.0 was used to solving the governing equations.

However, Muhammad [30], who studied the reactor (FCC riser) using alumina as a catalyst, employed the used FLUENT 6.3 for discretization, meshing, and governing equations solution. A similar approach was employed by Xiaomin et al. [39], unlike Rodrigo and Rosa [40], who employed the use of Fluent 6.1, Gambit, and PC-Simple, to obtained accurate results.

6. Turbulence Modelling as a Means of Enhancing Studies in Catalysis

The use of turbulence modeling has further enhanced studies and reveals several pieces of information in catalysis. Several forms of research works have been conducted to contribute to the promotion of better understanding in the field of modeling catalytic reaction systems. Some of the recent works carried are reported, as shown below.

Christoph et al. [29] employed the computational fluid dynamics approach to undertake an empirical and numerical study of the air-hydrogen catalytically stabilized combustion (CST) over platinum (Pt) catalyst in a turbulent flow. This was to assess the viability of applying CST in different near-wall turbulence representative equations and gain insight into the combination of turbulence and hetero/homo-gaseous burning processes. The examination of the turbulence in the CST of the hydrogen-air mixture in the Pt-covered passages demonstrated the significance of near-wall turbulence equations. This captures the inducement of laminarization with strong-flow through the heat transferred via the catalyst filled walls. It was established that the size of turbulent transport was central to the appraisal of catalytic fuel conversion and the homogeneous ignition process.

The result obtained inspired further studies by Christoph et al. [29]. One of the studies was focused on forecasting with three separate low Reynolds number (LRe) turbulence representative equations (coiled directly from the literature). This finding showed that for specific turbulence representative equation, they have keen sensitivity for hetero-/homogeneous processes

Christoph et al. [29] further reported that a steady flow laminarization decreases the conversion of the fuel by use of catalyst, and it also aids the start of uniform ignition. So, a rise in the rates of turbulent transport gives rise to incomplete fuel combustion in the gaseous zone, leaked fuel conversion using catalysts, and finally, to flame extermination. However, the experimental studies of Christoph et al. [29] show that the model of Ezato reproduces with good accuracy both for the pre-ignition catalytic conversion and the onset of homogeneous ignition, although it overpredicted the degree of orderliness or laminarization mildly.

Rodrigo and Rosa [40] studied the use of CFD software for modeling turbulence in two or more phase flows inside TBRs under high pressure. However, the report shows that the use of CFD for single-phase reactors are a successful tool. So, the authors examined the use of CFD for exemplifying three-dimensional (3-D) interstitial flow in a reactor with two or more phases through the influence of fluctuating turbulent velocities and non-directional quantities for the multiphase (MTP) flow. In their studies, the effects of representative equations for turbulence in two or more phase flows were evaluated. An Euler-Euler representative equation was then evolved, and various RANs models such as realizable, standard, and RNG k-ε representative equations, including the RSM for the computer-aided simulation of hydrodynamics of the TBR under high pressure. The report showed that several analyses were executed for the study of the characteristics in the search for numerical solution parameters. This was because the

simulation accuracy frequently depended on the density of the mesh, sizes of the mesh, time interval, conditions for convergence, and schemes for unique identification. The various solutions for the hydrodynamic confirmation of the MTP flow model were compared, and it was identified that the CFD forecast with the monotonic upwind scheme for conservation laws (MUSCL) scheme agreed well with the data obtained from experiments. The findings were the results of the total variation diminishing (TVD) algorithm, which superseded the numerical dispersion displayed in the simulation of two or more-phase flows. The optimum conditions obtained were employed in the determination of the various RANS turbulence representative equations. Here, it was identified that a temperature rise resulted in evenness of fluid mal-distribution inside the packed bed. It confirmed that better agreement was achieved with standard k-ε and RSM representative equations for the multi-phase trickle bed reactors.

In 2010, Binxin [41] evaluated different turbulence models. These include the three (3) HRe k-ε representative equations, six (6) LRe k-ε representative equations, two (2) k-ω representative equations, and the RSM for a single-phase non-Newtonian fluid flow in anaerobic digesters. This was achieved by relating the pressure drops obtained from the study of the process's CFD. The findings from the simulation conducted unveil that the Chang-Hsieh-Chen account of the LRe k-ε representative equation gave superior efficiency compared to other representative equations in the prediction of the pressure losses. In contrast, the standard k-ω representative equation had a low computing cost and acceptable accuracy, which agreed with Rodrigo and Rosa [40].

Muhammad [30] simulated FCC riser using the model (k-e), three different mesh, and three lump kinetic models to studies the two-phase flow of vapor and catalyst to describe the profiles of temperature, mass fraction, and the gasoline product yield within the reactor (FCC riser). The finding shows that all the simulation results did not unveil any significant difference for different mesh sizes, which was not in agreement with the report of Rodrigo and Rosa [40] for the use of different mesh sizes to enhance accurate predictions.

It was further deduced that the wrong selection of kinetic models could also contribute to poor prediction. This was because Muhammad [30] deduced that the setback of three lump kinetic representative equations could not forecast the mole fraction of coke and low molecular weight gases separately. However, Muhammed [43] in 2015, further the study on the FCC riser, where the use of four lump kinetic models was employed to solve the problem reported in Mohammed [30]. Both Muhammad's studies [30, 43] predict that the most complex segment of an FCC rise is the inlet zone. Although, Muhammed [21] reported that the reaction holds in the initial 2–4

m of the length of the FCC riser, while Muhammed [43] reported that in the first 1 – 3 m. The difference in the prediction was due to the different kinetic models used. However, both works reported that the plant data and model results agree quite well, especially when more realistic kinetic parameters are incorporated [43, 44]. The model that is proposed finds usage in all FCC riser simulation processes.

Xiaomin et al. [39] modeled a 2D – CFD for a fixed-bed (FB) reactor that uses a catalyst to remove hydrogen from syngas. The study simulated the flow behavior across the bed of catalyst. The modeling involves the combination of the CFD model for a porous medium with a reaction kinetics model. This approach enables the study to identify a more efficient kinetics model, which could better predict the reaction profile in the presence of the catalyst. With the use of the reaction mechanism and a statistical test, the study was able to identify a reliable representative equation for kinetics with separation–adsorption of oxygen gas molecules, which indicates the rate-controlling step. This step was identified and validated. The CFD model of the porous medium, in addition to a representative equation for kinetics, could give results of a simulation that agrees well with data from empirical studies. It was observed that the space velocity had a lower influence on the reaction, with appreciable values of space velocity given in the range of 2000–2200 h^{-1}.

Also, the CFD representative equation was used to forecast the distributions of the primary reaction variable. These variables include the concentration of the reacting species and the temperature within the reactor. H_2 conversion and hotspot temperature were greatly influenced by the inlet gas temperature and less by the inlet H_2 concentration, which should be kept below 1.4 % to eliminate temperature runoff. The flow rate of O_2 in the reactor is a dependent variable that can ensure that the expected conversion and desirable hot spot temperature are achieved [39].

Dominick et al. [31] determined the extent of mal-distribution of flows within the bed of the catalyst using COMSOL Multi-physics and a 2-D axis-symmetric model. They also evaluated the influence of flow's direction, size of the catalyst pellet, total and different screen opposition, and the overall volume of flow passing inside the reactor. This study reveals that the catalyst with a diameter of 1/8" allowed increased bed velocity and flow rate at a specific pressure loss. However, a faster flow volume could be advantageous. The increased bed velocity implies that the residence time of the fluid in the catalyst bed will be reduced, and reaction conversion is minimized. Results also give values for the index of maldistribution that hints that the 1/16" catalyst gives superior distribution in the catalyst bed. Dominick et al. [31] indicated that the

particle size of the catalyst would be the critical factor in determining the distribution of flows in the catalyst bed center. An enhanced distribution within the catalyst bed positively promotes the conversion process and the reactor's efficiency. Hence, this revealed that the 1/16" catalyst is preferred in the modeled reactor since it promotes higher reactor efficiency.

Zhapbasbayev et al. [42] modeled the turbulent flow within a radial fixed bed reactor using the k-e model, employing a unified approach for writing the motion equation for the numerical solution of the problem in a hybrid region. However, the computational study signifies that the flow within the fixed bed results in the generation of the kinetic energy of turbulence fluctuation and its rate of gradual disappearance. The patterns of the kinetic energy of turbulence fluctuation and its rate of gradual disappearance show the similarity of all turbulent characteristics in terms of the Reynolds number estimation.

Afshin [32] evaluated the effect of carbon tetrachloride (CCl_4) addition as propulsion to the thermal cracking reactor due to the quantity of coke formed in various COT. The findings identified that the *k-ε* realizable model would best predict turbulence behavior in a cracking process. Arising from this research and in collaboration with other reports showed that the optimum volume of CCL_4 that ensures fixed conversion was 100 ppm, and beyond this value, the process will be uneconomical.

7. Conclusions

Turbulent flow is said to be a flow zone or space in fluid dynamics characterized by disorganized changes in velocity and pressure of the flow. It contrasts, a flow regime which holds when fluid flows in parallel layers, with negligible disturbance in the layers is referred to as laminar flow. Meanwhile, this study indicates that as the pore size of the catalyst becomes more extensive, the speed of reaction drops responsively. It can so be said that the larger the turbulence eddies in the reactant flow stream, the lower the speed of reaction. Also, this review shows that models like K–ε, and RSM turbulence model will be useful for the prediction or study of turbulence behavior in a catalytic reaction. It was identified that selecting the appropriate turbulence model in a kinetic study plays a vital role in promoting accurate reaction kinetics prediction when carrying out the simulation.

However, this study identifies that only a few research works give attention to the right or appropriate use or selection of a kinetic model for catalytic reaction systems. Besides, it was also identified that there are little works that employed the study of whether the S-a model could enhance better prediction in the modeling of turbulence in a catalytic reaction system.

8. Recommendations

It is recommended that further studies should consider the accuracy of predictions of catalytic reaction systems when using the *s-a* turbulence model. Attention may also be given to the study of the best approach to selecting the correct kinetic model of a catalytic system, and the effect of using incorrect or inappropriate kinetic models.

9. Acknowledgments

The first author wishes to acknowledge to support of the PTDF in making the program successful.

10. References

[1] G. K. Batchelor. *An introduction to fluid dynamics*, Cambridge, University Press, 2000.
[2] H. Tennekes, J.L. Lumley, L.J. Lumley. *A first course in turbulence*. Cambridge, MIT Press, 1996.
[3] F. C. K. Ting, J. T. Kirby. Dynamics of surf-zone turbulence in a spilling breaker, *Coastal Engineering*, vol. 27(3–4), pp. 131–160, 1996.
[4] E. Kunze, J. F. Dower, I. Beveridge, R. Dewey, K. P. Bartlett. Observations of biologically generated turbulence in a coastal inlet. *Science*, vol. 313 (5794), pp. 1768-1770, 2006.
[5] I. Eames, J. B. Flor. *New developments in understanding interfacial processes in turbulent flows.* Royal Society Publishing, 2018. http://rsta.royal societypublishing.org, accessed on 21 January 2018.
[6] S. H. Strogatz. *Nonlinear dynamics and chaos: with applications to physics, biology, chemistry, and engineering*. Florida, CRC Press, 2018.
[7] H. G. Schuster, W. Just. *Deterministic chaos: an introduction*. Hoboken, John Wiley & Sons, 2006.
[8] S. T. Sie. Past, present, and future role of microporous catalysts in the petroleum industry. *Studies in Surface Science and Catalysis,* vol. 85, pp. 587-631, 1994.
[9] C. Bartholomew. Catalyst deactivation/ regeneration. *Encyclopedia of Catalysis,* 2002.
[10] C. H. Bartholomew, R. J. Farrauto. *Fundamentals of industrial catalytic processes*. John Wiley & Sons, 2011.
[11] Chemguide, Guide, https://www.Chemguide.co.uk/phys ical/basicrates/catalyst.html, accessed on 31 May 2018.
[12] T. Kuwabara, P. Kurzweil. Fuel Cells–Phosphoric Acid Fuel Cells | Anodes, *Encyclopedia of Electrochemical Power Sources,* p. 548-556, 2009.
[13] T. Oyegoke, F. N. Dabai, U. Adamu, B. E. Y. Jibril. Density functional theory calculation of propane cracking mechanism over chromium (III) oxide by cluster approach. *Journal of the Serbian Chemical Society,* vol. 85(5), pp. 1-14, 2020.
[14] H. Knözinger, K. Kochloefl. *Heterogeneous Catalysis and Solid Catalysts,* Ullmann's Encyclopedia of Industrial Chemistry, Wiley-VCH, Weinheim, 2002. DOI:10.1002/14356007.a05_313
[15] G. Vicente, M. Martınez, J. Aracil. Integrated biodiesel production: a comparison of different homogeneous catalysts systems. *Bioresource Technology,* vol. 92(3), pp. 297-305, 2004.
[16] T. C. Johnson, D. J. Morris, M. Wills. Hydrogen generation from formic acid and alcohols using homogeneous catalysts. *Chemical Society Reviews*, vol. 39(1), pp. 81-88, 2010.

[17] Z. Helwani, M. R. Othman, N. Aziz, J. Kim, W. J. N. Fernando (2009). Solid heterogeneous catalysts for transesterification of triglycerides with methanol: a review. *Applied Catalysis A: General*, vol. 363(1-2), pp. 1-10.

[18] T. Oyegoke, F. N. Dabai, U. Adamu, B. E. Y. Jibril. Insight from the study of acidity and reactivity of Cr_2O_3 catalyst in propane dehydrogenation: a computational approach. *Bayero Journal of Pure and Applied Sciences*, vol. 11(1), pp. 178-184, 2018.

[19] Y. Zhao, K. R. Yang, Z. Wang, X. Yan, S. Cao, Y. Ye, K. L. Materna. Stable iridium dinuclear heterogeneous catalysts supported on the metal-oxide substrate for solar water oxidation. *Proceedings of the National Academy of Sciences*, 201722137, 2018.

[20] S. Morales-Delarosa, J. M. Campos-Martin, J. L. Fierro. Chemical hydrolysis of cellulose into fermentable sugars through ionic liquids and antisolvent pre-treatments using heterogeneous catalysts. *Catalysis Today*, vol. 302, pp. 87-93, 2018.

[21] J. Gao, Y. Wang, Y. Du, L. Zhou, Y. He, L. Ma, Y. Jiang. Construction of biocatalytic colloidosome using lipase-containing dendritic mesoporous silica nanospheres for enhanced enzyme catalysis. *Chemical Engineering Journal*, vol. 317, pp. 175-186, 2017.

[22] D. C. Cubides-Roman, V. H. Pérez, H. F. de Castro, C. E. Orrego, O. H. Giraldo, E. G. Silveira, G. F. David. Ethyl esters (biodiesel) production by Pseudomonas fluorescens lipase immobilized on chitosan with magnetic properties in a bioreactor assisted by an electromagnetic field. *Fuel*, vol. 196, pp. 481-487, 2017.

[23] R. Das, M. Talat, O. N. Srivastava, A. M. Kayastha. Covalent immobilization of peanut β-amylase for producing industrial nano-biocatalysts: A comparative study of kinetics, stability, and reusability of the immobilized enzyme. *Food Chemistry*, vol. 245, pp. 488-499, 2018.

[24] J. Matthiesen, S. Wendt, J. O. Hansen, G. K. Madsen, E. Lira, P. Galliker, E. K. Vestergaard, R. Schaub, E. Laegsgaard, B. Hammer, F. Besenbacher. Observation of All the Intermediate Steps of a Chemical Reaction on an Oxide Surface by Scanning Tunnelling Microscopy. *ACS Nano.*, vol. 3(3), pp. 517–526, 2009.

[25] M. E. Davis, R. J. Davis. *Fundamentals of Chemical Reaction Engineering*, New York, McGraw-Hill Company, 2003.

[26] H. S. Fogler. *Essentials of chemical reaction engineering*. 4th Edition, Westford, MA, Pearson Education, 2006.

[27] B. Andersson. *Computational fluid dynamics for engineers*, Cambridge, Cambridge University Press, 2012.

[28] J. C. Ching, J. Sheng-Yuh. *Fundamentals of turbulence modeling*, Abingdon, Taylor & Francis, 1998.

[29] A. Christoph, J. Mantzaras, R. Schaeren, R. Bombach, A. Inauen, B. Kaeppeli, A. Stampanoni. An experimental and numerical investigation of homogeneous ignition in catalytically stabilized combustion of hydrogen/air mixtures over platinum. *Combustion and Flame*, vol. 128(4), pp. 340-368, 2002.

[30] A. Muhammad. Computational fluid dynamics (CFD) prediction of mass fraction profiles of gas oil and gasoline in fluid catalytic cracking (FCC) riser. *Ain Shams Engineering Journal*, vol. 3(4), pp. 403-409, 2012.

[31] T. I. Dominick, I. E. Specht. *Experimental and Numerical Analysis of Flow Mixing in Packed Beds*, Doctoral Thesis, Otto von Guericke University, Magdeburg, 2016.

[32] D. Afshin. Evaluation of Adding Carbon Tetrachloride as Propulsion to the Thermal Cracking Reactor due to the Amount of Formed Coke in Different Coil Outlet Temperatures (COT). *J. Thermodyn. Catal.*, vol. 8(179), pp. 2, 2017.

[33] W. Rodi. *Turbulence models and their application in hydraulics*. Florida, CRC Press, 2017.

[34] J. Sodja. *Turbulence models in CFD*, Technical Report, University of Ljubljana, Ljubljana, pp.1-18, 2007.
[35] S. S. Girimaji. Pressure–strain correlation modeling of complex turbulent flows. *Journal of Fluid Mechanics*, vol. 422, pp. 91-123, 2000.
[36] C. Stephen, D. Caraeni, L. Fuchs. Large-eddy simulation of the flow through the blades of a swirl generator. *International journal of heat and fluid flow*, vol. 21(5), pp. 664-673, 2000.
[37] J. Lumley, G. Newman. The return to isotropy of homogeneous turbulence, *Journal of Fluid Mechanics*, vol. 82, pp. 161–178, 1977.
[38] A. Mishra, S. Girimaji. Intercomponent energy transfer in incompressible homogeneous turbulence: multi-point physics and amenability to one-point closures, *Journal of Fluid Mechanics*, vol. 731, pp. 639–681, 2013.
[39] X. Xiaomin, J. Dai, Z. Luo. CFD modeling using heterogeneous reaction kinetics for catalytic dehydrogenation syngas reactions in a fixed-bed reactor. *Particuology*, vol. 11(6), pp. 703-714, 2013.
[40] L. J. Rodrigo, F. M. Rosa-Quinta. Turbulence modeling of multiphase flow in high-pressure trickle-bed reactors. *Chemical Engineering Science*, vol. 64(8), pp. 1806-1819, 2009.
[41] W. Binxin. Computational fluid dynamics investigation of turbulence models for non-Newtonian fluid flow in anaerobic digesters. *Environmental science & technology*, vol. 44(23), pp. 8989-8995, 2010.
[42] U. K. Zhapbasbayev, G. I. Ramazanova, O. B. Kenzhaliev. Modeling of turbulent flow in a radial reactor with a fixed bed, *Thermophysics and Aeromechanics*, vol. 22(2), pp. 229-243, 2015.
[43] A. Muhammed. Prediction of gasoline yield in a fluid catalytic cracking (FCC) riser using k-epsilon turbulence and 4-lump kinetic models: A computational fluid dynamics (CFD) approach. *Journal of King Saud University-Engineering Sciences*, vol, 27(2), 130-136, 2015.
[44] A. Gianetto, H. I. Farag, A. P. Blasetti, H. I. de Lasa. Fluid catalytic cracking catalyst for reformulated gasoline. Kinetic modeling. *Industrial & engineering chemistry research*, vol. 33(12), pp. 3053-3062, 1994.