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Modeling of Single Channel Monolithic Reactor with The Single pass Flow Operation System

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Abstract

In the following sections, the recent published studies on modeling and simulation of monolith reactors were reviewed Mass transfer, and reaction kinetics were achieved by establishing mass, energy and momentum balance equations. The model equations were solved simultaneously. Such a model can be useful for studying the impact of changes of superficial gas and liquid velocities on reaction rate within the slug flow regime.The reaction system used is the hydrogenation α–methyl styrene (AMS) to cumene over a palladium on γ–alumina catalyst, It is a well known system used to understand three-phase reactor performance under mass transfer limited condition by the gas mass transfer through the liquid film at the catalyst surface to the active sites. The effects of superficial gas and liquid velocities on reaction rate were studied with the range of 10 cm/s≤ UL ≤ 30 cm/s, and 10 cm/s ≤ UG ≤ 30 cm/s. The flow pattern for all these range of velocities was in the Taylor flow pattern.

Keywords: Hydrogenation; Hydrodynamics; Mass Transfer; Kinetic model; Modeling; Monolithic reactor.

نمذجة المفاعل المونولوثي وحيد القناة بنظام جريان الممر الواحد

ألخلاصه

في هذه الدراسه تم اجراء عرض للدراسات المنشوره الحديثه عن نمذجة وتمثيل مفاعلات المونولث. انتقال الكتله و حركية التفاعل يمكن التوصل اليها من خلال معادلات موازنة الكتله, الحرارة والزخم. حلت معادلات الموديل بشكل اني, مثل هذا النموذج يمكن ان يكون مفيد لدراسة تأثير سرعة انتقال الغاز والسائل ضمن نظام تدفق (Slug flow regime). نظام التفاعل المستخدم هو هدرجة الفا مثيل ستايرين (AMS) الى الكيومين, فوق البلاديوم المحمل على الكاما الومينا كعامل مساعد, انه نظام معروف جيدا يستخدم لفهم اداء المفاعلات ثلاثية الطور تحت ظروف انتقال كتله محدده بانتقال الغاز خلال طبقة السائل الرقيقه على سطح العامل المساعد الى المواقع الفعاله. تأثير سرع الغاز والسائل على معدل التفاعل تم دراستها ضمن حدود 10 cm/s ≤ UL ≤30 cm/s, و 10 cm/s ≤ UG ≤30 cm. نوع الجريان لكل حدود السرع هذه هو نظام جريان (Taylor Flow Pattern).

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1- Introduction

In general, monolith reactors refer to reactors that contain catalysts with certain structures or arrangements. According to this definition, there are many different types of monolith reactors, such as honeycomb, foam, and fiber reactors, etc. Usually monolith reactors refer to those containing catalysts with parallel straight channels inside the catalyst block. The straight channels normally have circular, square or triangular cross-sections. Monolith catalysts or monolith reactors have some common features in most of the applications they are used for. These features or characteristics include: (1) low pressure drop especially under high fluid throughputs; (2)
elimination of external mass transfer and internal diffusion limitations; (3) low axial dispersion and back-mixing, and therefore high product selectivity; (4) larger external surface; (5) uniform distribution of flow (gas phase); (6) elimination of fouling and plugging, and thus extended catalyst lifetime; (7) easy scale-up, etc.

Monolith reactors were initially developed and applied to the automobile industry as vehicle engine emission converters to remove NOx and CO via fast gas phase reactions. Compared to the traditional catalysts used for gas phase reactions, monolith has obviously predominating advantages as mentioned above. These characteristics are favorable to the exhaust gas treatment, resulting in high selectivity and elimination of hot-spot, and promoting the conversion rate and reaction performance (Cybulski and Moulijn 1998). In the last two decades, the success of monoliths as engine emission converters has encouraged researchers to investigate how to improve other gas phase reactions by using monolithic catalysts and reactors. Such applications include catalytic combustion (Tischebr and Deutschmann 2005), catalytic oxidation (Boger and Menegola 2005), hydrogenation or dehydrogenation (Sadykov et al. 2000), and methanation (Sughrue and Bartholomew 1982). Some other gas phase applications of monoliths have been summarized by (Heck et al. 2001).

If gaseous and liquid reactants flow through catalytically active monoliths, complex physical and chemical phenomena take place at different scales of the reactor. At the smallest scale, the reactants diffuse, adsorb, react on the active sites, desorb and diffuse back into bulk fluid flow. Modeling the monolithic reactors comprises the contributions of reaction kinetics, external and intra particle mass transfer and hydrodynamics.

The monolithic reactors have been modeled by different researchers (Hatziantoniou et al. 1984; Irandoust et al. 1988; Cybulski et al. 1993; Edvinsson and Cybulski 1994 and 1995; Cybulski et al., 1999; Nijhuis et al., 2003; Kreutzer et al. 2005).

Hatziantoniou et al. (1984) investigated the hydrogenation of nitrobenzoic acid over palladium catalyst using monolithic reactor operating in slug flow regime.

Irandoust et al. (1988) developed a mass transfer model in which plug flow is assumed in the liquid phase. Three different mass transfer fluxes (G-L, G-S, L-S) are considered in the differential mass balance for reacting species.

Edvinsson and Cybulski (1994 and 1995) compared numerically the performance of a trickle-bed reactor and a monolithic reactor in terms of space-time yield, selectivity and pressure drop. They concluded that the monolithic reactor is characterized by a much lower pressure drop than trickle bed reactor.

Cybulski et al. (1999) performed a comprehensive theoretical analysis of a monolithic reactor and an agitated slurry reactor. In different case studies, it is shown that the monolithic reactor was greater compared with the slurry reactor.

Kreutzer et al. (2001) developed a model for modeling AMS hydrogenation in the monolithic reactor. They concluded that, although mass-transfer to the catalyst is somewhat limiting the reaction rate, the mass-transfer rates are close to the kinetically controlled rates, since the styrene and hydrogen concentrations near the catalyst surface are close to the bulk concentrations.

Nijhuis et al. (2003) evaluated theoretically the performance of a monolithic reactor and a trickle-bed reactor using the hydrogenation of styrene. The authors demonstrated that the monolithic reactor yields productivity which is three times greater, while using four times less catalyst.

Kreutzer et al. (2005) modeled the hydrogenation 2,4-dinitrotoluene using a monolithic loop reactor. It was concluded that the reactor should be operated at the lowest possible superficial liquid and gas velocities in stable slug flow regime In the same department Bauer 2007, studied experimentally the flow regimes and reactor performance of monolithic reactor with different catalyst beds and catalytic preparation methods.

From the previous research; it was found that little attention has been paid to the monolithic reactor modeling. Therefore this paper contains a study to provide a mathematical model for monolith reactor operated in co-current flow.

The hydrogenation of α-methyl styrene (AMS) to cumene is considered as model reaction. The effects of superficial gas and liquid velocities, in down flow mode with micro mixer gas-liquid distributor have been investigated. The model was formulated for single pass conversion of the liquid reactant (AMS) passing through the reactor. The model evaluation is done by comparing model predictions against experimental data by Adel (2008). The work provides a mathematical model of the monolithic reactor as well as numerical process simulations for a range ofoperating conditions. The proposed model is validated using experimental data

obtained from reaction experiments at different gas and liquid superficial velocities for slug flow pattern by Adel (2008). Furthermore, the influence of its on AMS conversion is studied.

2. Model Assumption

The developed model for the monolithic reactor is based on the following assumptions:

1- Gas and liquid flow in co-current constant flow rate.

2- Operation in the Taylor flow regime (Bauer 2007).

3- Isothermal operating condition of the reactor.

4- Liquid components are non-volatile.
5- Constant physical properties.
6- Steady state operation.
7- No radial and axial dispersion.
8- Uniform gas-liquid distribution over the channel cross-section.
9-Catalyst effectiveness 100% and no mass transfer resistance on the gas phase side.
10-Active sites are homogeneously in the washcoat layer.
(Nijhuis et al., 2003; Bauer et al., 2005; and Bauer, 2007)

3. Model Equations

3.1 Mass Balance

The mathematical reactor model developed in this work consists of mass balances of all species in the gas phase, liquid phase, and catalyst layer. Based on the assumptions described, the reactor model is given by the following set of equations for each phase.

A) AMS concentration in liquid bulk:

$$U_L \frac{\partial C_{A,b}}{\partial z} = k_{LS} a_{LS} (C_{A,c} - C_{A,b}) \quad ..(1)$$

B) Hydrogen concentration in liquid bulk:

$$U_L \frac{\partial C_{H,b}}{\partial z} = k_{LS,H} a_{LS} (C_{H,c} - C_{H,b}) + k_{GL} a_{GL} (C_{H,sat} - C_{H,b}) \quad .. (2)$$

C) AMS concentration at catalyst:

$$k_{LS} a_{LS} (C_{A,b} - C_{A,c}) = r_m \frac{4 d_{wc}}{d_C} \quad .. (3)$$

D) Hydrogen concentration at catalyst:

$$k_{LS,H} a_{LS} (C_{H,b} - C_{H,c}) + k_{GS} a_{GS} (C_{H,sat} - C_{H,c}) = r_m \frac{4 d_{wc}}{d_C} \quad ..... (4)$$

E) Hydrogen flow balance:

$$\frac{\partial f_H}{\partial z} = -k_{GL} a_{GL} (C_{H,sat} - C_{H,b}) - k_{GS} a_{GS} (C_{H,sat} - C_{H,c}) \quad ..(5)$$

3.2. Heat balance

$$\frac{\partial T}{\partial z} = \frac{r_m \frac{4 d_{wc}}{d_C} \Delta H_r}{U_L \frac{r_L Cp_L}{M_L} + U_G \frac{r_G Cp_G}{M_G}} \quad .. (6)$$

3.3 Hydrodynamic and mass transfer

In monolithic reactor model all external mass-transfer steps for both hydrogen and styrene are taken into account. The schematic representation of these individual mass-transfer steps are depicted in Figure 1. For the AMS mass-transfer from the bulk of the liquid (the slugs) to the catalyst surface is considered. For hydrogen both 'direct' mass-transfer from the gas bubbles through the thin liquid film to the catalyst surface and indirect mass-transfer from the gas bubbles via the liquid slugs to the catalyst surface are taken into account. Where, mass transfer coefficients are given by the following equations Irandoust and Andersson (1989):

$$K_{GS} = \frac{D_{H_2}}{d} \quad ..(7)$$

Natividad et al. (2007):

$$K_{LS} = 20 \frac{D_{H_2}}{d_c} \left[1 + 0.003 \left(\frac{y_{slug}}{\mathrm{Re}\, Sc} \right)^{-0.7} \right] \quad ..(8)$$

Kreutzer et al. (2001):

$$(K_{GL} a_{GL})_{H_2} = \frac{0.133 U_{TP}^{1.2}}{L_{Slug}^{0.5}} \left(\frac{D_{H_2}}{D_{CH_4}} \right)^{0.5} \quad .. (9)$$

where D_{CH4} = 5 X 10^{-9} m^2/s, and specific area:

$$a_{GS} = \frac{4(1-e_L)}{d_c} \quad \ldots (10)$$

And

$$a_{LS} = \frac{4 \in_L}{d_c} \quad \ldots.(11)$$

The hydrodynamic parameters:
Liquid slug length: Kreutzer et al. (2001).

$$L_{slug} = d_c \frac{e_L}{-0.00141 - 1.556 e_L^2 \ln(e_L)} \quad \ldots.(12)$$

Gas bubble length

$$L_B = L_{slug} \frac{1-e_L}{e_L} \quad \ldots (13)$$

Liquid film thickness: Irandoust and Andersson (1986).

$$d = 0.18 d_c \left[1 - \exp\left(-3.08 Ca^{0.54}\right)\right] \quad ..(14)$$

Gas bubble diameter:

$$d_B = d_c - 2d \quad ..(15)$$

Liquid hold up:

$$e_L = \frac{U_L}{U_{TP}} \quad .. (16)$$

where $U_{TP} = U_L + U_G$

The total mass transfer of H_2 in a monolith channel can be described by $N_T a_T$:

$$N_T a_T = N_{GS} a_{GS} + N_{LS} a_{LS} + N_{GL} a_{GL} \quad ..(17)$$

$$N_T a_T = \left[K_{GS} a_{GS} + \frac{K_{LS} a_{LS} K_{GL} a_{GL}}{K_{LS} a_{LS} + K_{GL} a_{GL}}\right]\left(C^*_{H_2} - C_{H_{2S}}\right) \quad \ldots.(18)$$

$$R_T = N_T a_T \quad \ldots(19)$$

$$K_{GS} a_{GS} + \left(\frac{1}{K_{GL} a_{GL}} + \frac{1}{K_{LS} a_{LS}}\right)^{-1} = K_{ov} a \quad \ldots(20)$$

Finally the surface concentration of hydrogen from equation (N_T a_T) is used to estimate the diffusional resistance

$$X_{LS} = \frac{C^*_{H_2} - C_{H_{2S}}}{C^*_{H_2}} \quad \ldots (21)$$

These equations were solved simultaneously in a process modeling and simulation software (Matlab) by using orthogonal collection method on finite.

3.4 Intrinsic Kinetics

The hydrogenation of α-methylstyrene were selected. The experimental investigation of the kinetics of the hydrogenation of α-methylstyrene was performed as illustrated in Adel (2008), and the intrinsic reaction rate was expressed as follow.

$$-r_S = \frac{k K_A K_{H_2} C_A C_{H_2}}{\left(1 + K_A C_A + \sqrt{K_{H_2} C_{H_2}}\right)^3} \quad \ldots.(22)$$

3.5 Pressure Drop

The monolithic structure shows a very low pressure drop in consequence of the straight channels and excellent mass transfer rates. Kreutzer (2003) defined a two-phase pressure drop according to equation (23).

$$DP_f = 4f\frac{L}{dc}\frac{1}{2}r_L(1-e_L)(U_L+U_G)^2 \quad \ldots(23)$$

Kreutzer et al. (2001) developed the correlation for friction factor.

$$f = \frac{16}{Re}\left[1 + 0.17\frac{dc}{L_{Slug}}\left(\frac{Re}{Ca}\right)^{0.33}\right] \quad \ldots(24)$$

4. Numerical Methods

A simple one-dimensional reactor model was used to predict its performance of the monolith reactor. This model takes into account both intra and surface concentration and temperature gradients. The balance equations arising from the model make up a system of ordinary differential equations which together with the inlet conditions become an initial value problem.

The model Equations (1) to (5) were solved using MATLAB program. A finite difference formulation was used to solve model equations. The mass-transfer coefficients for both hydrogen and styrene are calculated by using Equations (7) to (16). Equations (23) and (24) were solved to calculate the pressure drop within the monolith reactor.

5. Results and Validation of the Reactor Model

Figure 2 represents a plot for the AMS conversion at different values of superficial gas and liquid velocity. By comparing the simulated AMS conversion with the experimental conversions for Adel (2008), the proposed model has been validated by comparing the calculated results with the experimental results.

6. Model Results and Discussion

The rate of reaction increased with the increase of hydrogen flow rate due to the increase of bubble length and the increase Gas-Solid mass transfer coefficient (See Figure 2).

The monolithic reactor is able to convert more reactant liquid to the product; it can be explained by the much more efficient mass transfer. As a result of the more efficient mass transfer the hydrogen concentration at the monolithic catalyst is high. This high concentration makes the catalyst is utilized much more effective. Is high effect is further illustrated by the fact that the monolithic reactor is able to achieve high productivity.

The absence of dry or stagnant liquid zones in the monolithic reactor is also an advantage, since all of the catalyst in the reactor is thereby being used and not subjected to different conditions. An added advantage for the monolithic reactor is that one would expect that the catalyst deactivation by gum formation on the catalyst would be much less for the monolithic catalyst, since gum-formation is prevented by a large hydrogen concentration on the catalyst (Moulijn et al. (2001)) (See Figure 3).

The concentration of AMS is reduced along the reactor length because it was

consumed by the reaction to produce cumene (See Figure 4). Therefore the AMS conversion is increased along the length of reactor (See Figure 5).

The hydrogenation reaction is an exothermic process (ΔH= -109 kJ/mol), the higher flow rates for gas and liquid and the absence of stagnant zones make the development of hot spot in a monolithic reactor considerably less (See Figure 6).

From Equations (23) and (24), a linear increase in pressure drop with gas and liquid flow rates. In general the pressure drop through the channels of monolith was very less, and therefore it can be neglected (See Figure 7). The reactor parameters used for modeling of monolith reactor can be shown in Table 1.

The real situation in the monolith channel is quite dynamic and complex with passing liquid slugs and gas bubbles, it is not necessary to model all the separate bubbles and slugs with a lot of changing boundary conditions at the catalyst. This is true since the liquid film which continuously wets the catalyst dampens out these rapid fluctuations making it possible to operate at close to a quasi steady-state (Edvinsson and Moulijn (1997)). Figure 8, shows the reaction solution algorithm.

Conclusions

It was confirmed that the developed channel by channel description of monolith honeycomb reactors is numerically tractable on fast workstation.

A one-dimensional reactor model was used to predict the performance of the monolith reactor. This model takes into account both intra and surface concentration and temperature gradients. The balance equations arising from the model make up a system of ordinary differential equations which together with the inlet conditions become an initial value problem. The model equations were solved using MATLAB program. A finite difference formulation was used to solve model equations.

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Nomenclatures

A	α-methyl styrene.
a	Specific interfacial area, (m^2/m^3).
C	Concentration, (mol/m^3).
C_{H2S}	Hydrogen concentration at the catalytic surface, (mol/ m^3).
Cp	Specific heat of a component, (kJ/kmol. K)
d	Diameter, (m).
D	Diffusivity, (m^2/s).
E_A	Activation energy, (kJ/mol)
f	Friction factor, (-).
H	Enthalpy, (KJ/mol).
K	Mass transfer coefficient, (m/s).
K	Equilibrium coefficient in the equation of reaction rate, (mol/gm min)
K	Equilibrium coefficien
k_{H2}	Constant for hydrogen adsorption, (1/s).
k_o	Pree exponential factor, (mol/gm.min)
M	Molecular weight, (gm/mol)
N	Mass flux, (mol/m^2).
P	Pressure, (bar).
ΔP	Pressure drop, (bar).
R	Gas constant, (pa. m^3/mol.K).
-r	Rate of reaction, (mol/m^3.s).
T	Temperature, K.
t_w	Wall thickness, (mm)
U	Superficial velocity (cm/s)
$X_{L.S}$	Liquid-solid mass transfer resistance, (-).

Greek Letters

ρ	Density, (kg/m^3).
Δ	Difference
ψ_{slug}	Dimensionless liquid slug length, (-).
μ	Dynamic viscosity, (kg/m s).
δ	Liquid film thickness, (mm).
σ	Surface tension, (N/m).
$\in$	Phase hold up, (-).

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ϕ	Volumetric flow rate, (m^3/s)

Subscripts

*	Equilibrium
A	α-methyl styrene
ads.	Adsorption
B	Bubble
b	Bulk
c	Channel
C	Cumene
CH_4	Methan
cat	Catalyst
eff	Effective
exp.	Experiment
G (or) g	Gas
GL	Gas-liquid
GS	Gas-solid
H_2	Hydrogen
i	Component i
int.	Intrinsic
L (or) l	Liquid
LS	Liquid-solid
m	monolith
o	Initial
ov	Over all
r	reaction
s	Surface
S	Solid
sat	Saturation
SL	Superficial liquid
T	Total
TP	Two phase
UC	Unit cell
wc	washcoat

Abbreviations

AMS Alpha methyl styrene

Dimensionless Numbers

Ca Capillary number = $\frac{mU}{s}$ (-)

Re Renold number = $\frac{r U d}{m}$ (-)

Sc Schmidt number = $\frac{m_L}{r_L D_i}$ (-)

Table (1) Reactor parameters used for modeling of monolithic reactor

Pressure (bar)	**10**
Liquid inlet temperature (K)	**383**
AMS concentration (mol/l)	**6.68**
Channel diameter (mm)	**1**
Channel length (cm)	**60**
Pd on catalyst (wt%)	**1.8%**
void fraction	**0.7**
cell density(CPSI)	**400**
Superficial liquid velocity (m/s)	**0.1-0.3**
Superficial gas velocity (m/s)	**0.1-0.3**

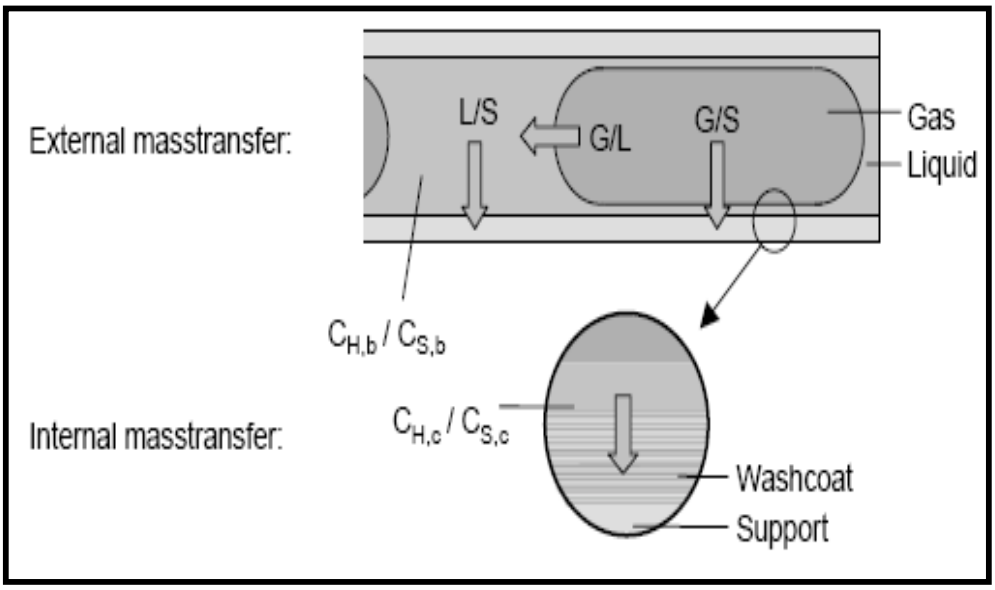

Figure (1) Schematic representation of the mass-transfer steps in a monolithic reactor.

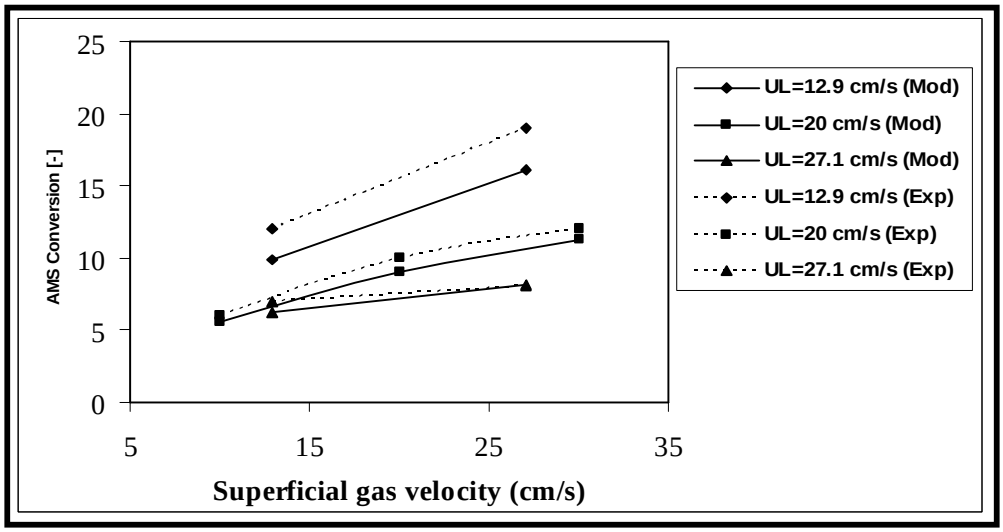

Figure (2) Validation between Experiment and Model results (Micro-Mixer distributor, Downflow, P=10 bar , T=110°C , C_{AMS_o}=6680 mol/m^3).

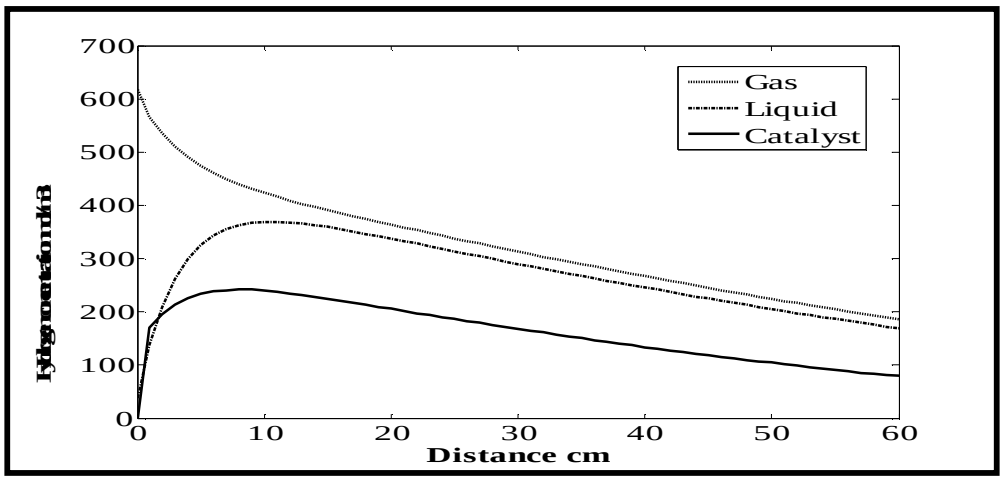

Figure (3) Hydrogen concentration profile in a monolithic reactor. (P=10 bar , T=110 ˚C , C_{AMS_0}=6680 mol/m^3 , U_L=10 cm/s , U_G=30 cm/s).

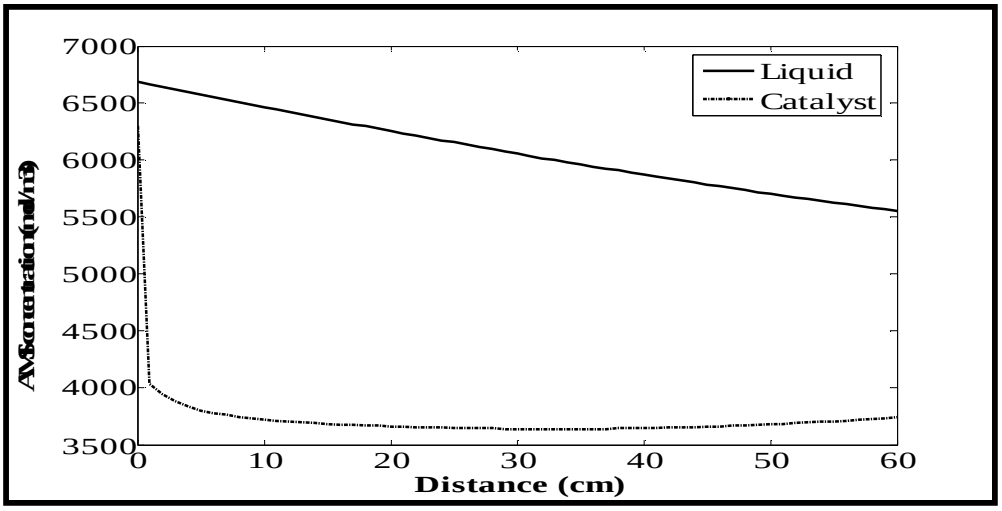

Figure (4): AMS concentration profile in a monolithic reactor. (P=10 bar, T=110 ºC, C_{AMS_0}=6680 mol/m^3, U_L=10 cm/s, U_G=30 cm/s).

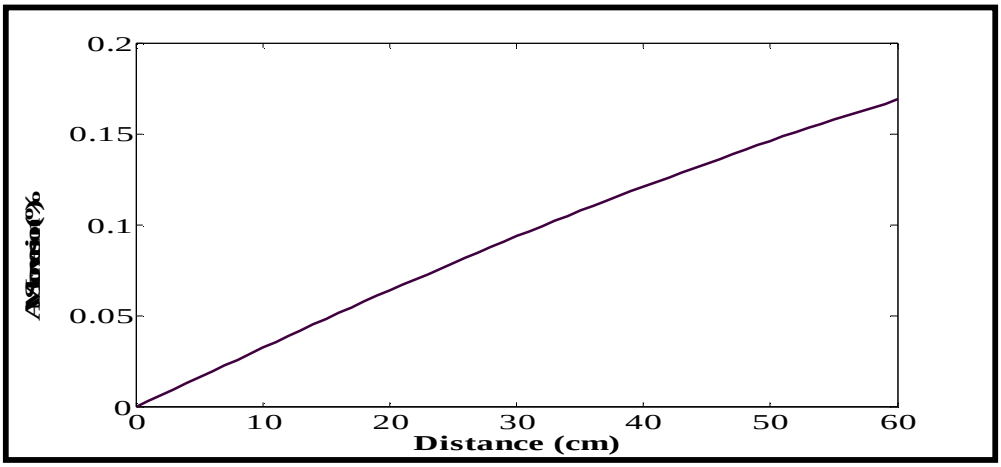

Figure (5): AMS Conversion along the monolith reactor.
(P=10 bar, T=110 ºC, CAMSo=6680 mol/m3 , UL=10 cm/s , UG=30 cm/s)

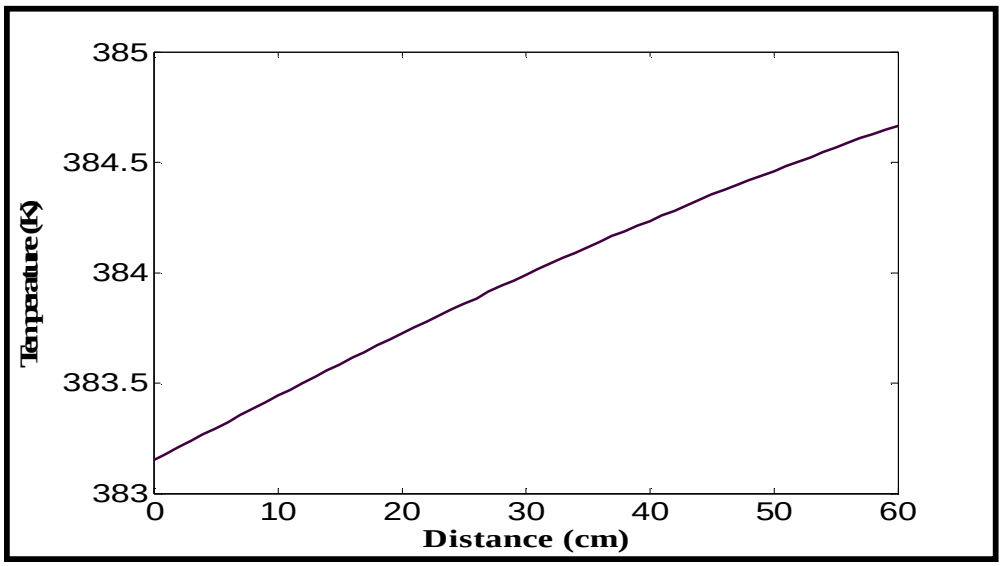

Figure (6): Temperature profile along the monolith reactor.
(P=10 bar, T=110 ˚C, CAMSo=6680 mol/m3 , UL=10 cm/s , UG=30 cm/s)

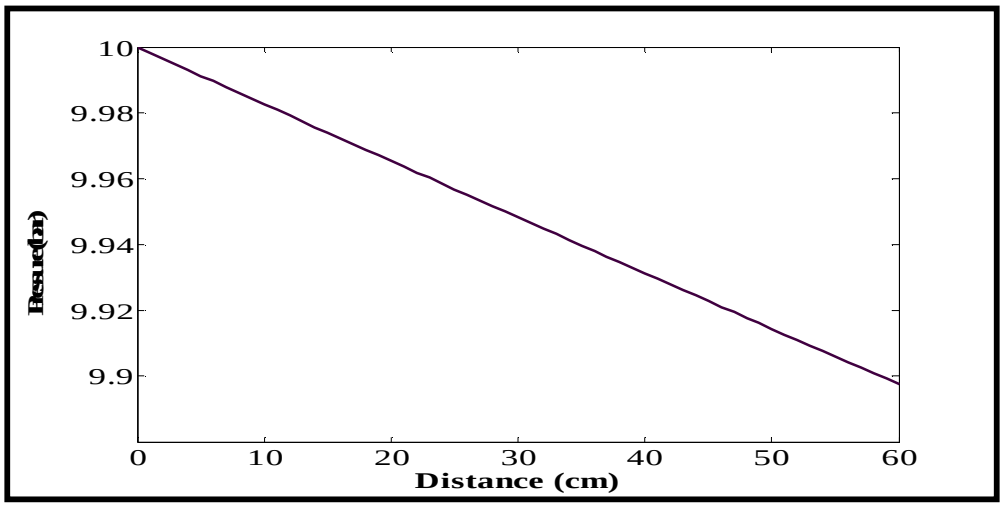

Figure (7): Pressure profile along the monolith reactor.
(P=10 bar, T=110 ˚C, CAMSo=6680 mol/m3 , UL=10 cm/s , UG=3.

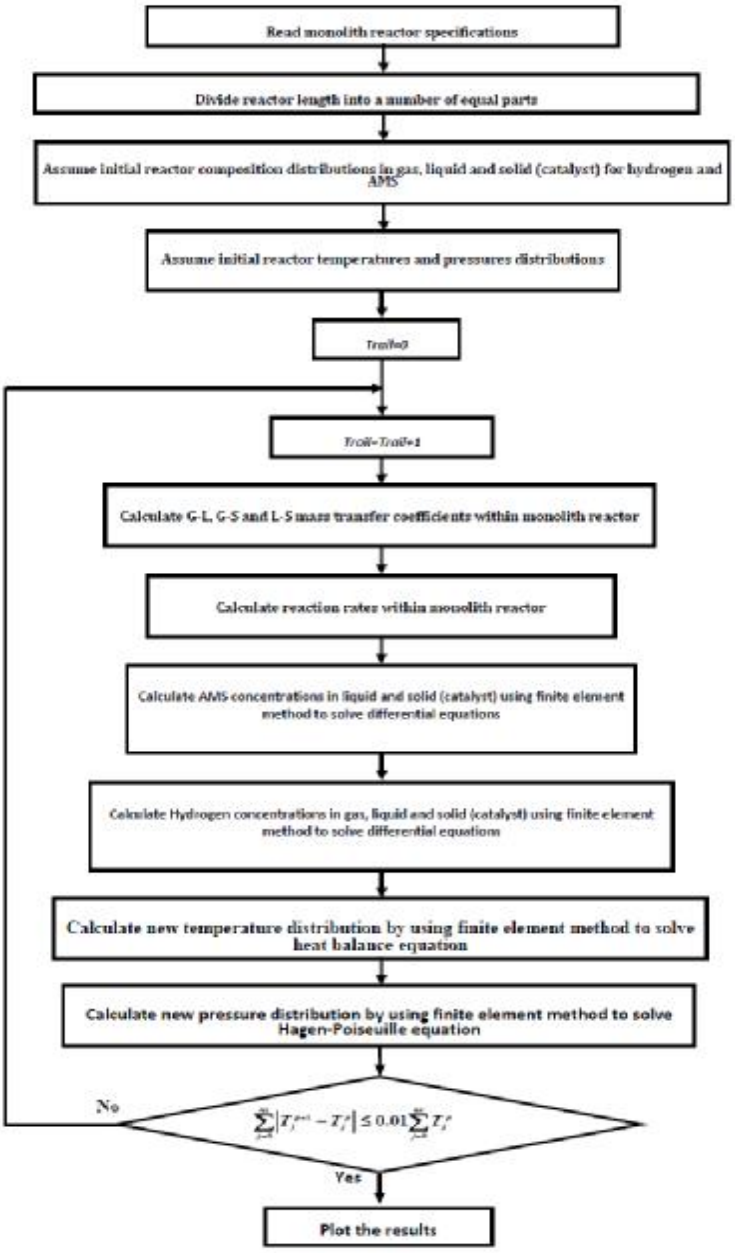

Figure (8): Reaction solution algorithm.