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Application of Hypergeometric Functions in Obtaining Space- Time Relationships for Steady State Plug Flow Reactor

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Abstract: This paper aims at the analysis of reactions for the special case of complete conversion (order $\neq$ 0, 1), occurring in a steady-state plug flow reactor.Hypergeometric function and later the Gauss's π - function, are employed to develop a generalized relationship between the space-times for two different ordered reactions. Further, the working techniques with these relationships are also indicated briefly.

Keywords: Degree of Conversion, Gauss's π - function ,Hypergeometric function, Order of the Reaction, Space-Time.

1 Introduction

The space-time 'τ 'is the proper performance measure for the flow reactors. It is defined as the actual time required to process one reactor volume of feed measured at specified conditions and has the unit of time.

For a steady-state plug flow reactor, the space-time is evaluated by the expression given by O. Levenspiel [11], as;

$$\tau = C_{A0} \int_{x_A=0}^{x_A} \frac{dx_A}{-r_A} \qquad \text{...... (1.1)}$$

where x_A is the degree of conversion, which is the ratio of moles of reactant converted; to the moles of reactant initially present.

For an unimolecular type n^{th} order reaction ($n \neq 0,1$) and constant density system; equation (1.1) may be written as

$$\tau_n = C_{A0} \int_{x_A=0}^{x_A} \frac{dx_A}{k_n C_A^n} \qquad \text{...... (1.2)}$$

For a constant density system, we have

$$C_A = C_{A0}(1 - x_A) \qquad \text{...... (1.3)}$$

Thus, equation (1.2) takes the form

$$\tau_n = C_{A0}\int_{x_A=0}^{x_A} \frac{dx_A}{k_n[C_{A0}(1-x_A)]^n} \qquad \text{...... (1.4)}$$

Equation (1.4) on further simplification yields

$$\tau_n = \frac{1}{k_n C_{A0}{}^{n-1}(n-1)}\left[\frac{1}{(1-x_A)^{n-1}} - 1\right] \qquad \text{...... (1.5)}$$

$$\Rightarrow (1-x_A)^{1-n} = \left\{\tau_n k_n C_{A0}{}^{n-1}(n-1)\right\} + 1 \qquad \text{...... (1.6)}$$

Or

$$(1-x_A)^{n-1} = \frac{1}{\left\{\tau_n k_n C_{A0}{}^{n-1}(n-1)\right\} + 1} \qquad \text{...... (1.7)}$$

For, $x_A = 1$; equation (1.6) and equation (1.7) gives unsatisfactory results and are thus worked upon further.

Thus, Hypergeometric series serves as the best mathematical tool to deal with this situation.

We now express equation (1.6) and equation (1.7) in terms of Hypergeometric function.

[2] Representation in Terms of Hypergeometric function

The Hypergeometric function is defined by A.R. Forsyth [4], as

$$F(\alpha,\beta;\gamma;x) = \left\{1 + \frac{\alpha\beta}{1.\gamma}x + \frac{\alpha(\alpha+1)\beta(\beta+1)}{1.2.\gamma(\gamma+1)}x^2 + \frac{\alpha(\alpha+1)(\alpha+2)\beta(\beta+1)(\beta+2)}{1.2.3.\gamma(\gamma+1)(\gamma+2)}x^3 + ...\right\} \qquad \text{...... (2.1)}$$

$$F(n-1,a;a;x_A) = \left\{\tau_n k_n C_{A0}{}^{n-1}(n-1)\right\} + 1 \qquad \text{..... (2.2)}$$

Similarly, equation (1.7) can be expressed in terms of Hypergeometric function as

$$F(1-n,b;b;x_A) = \frac{1}{\left\{\tau_n k_n C_{A0}{}^{n-1}(n-1)\right\} + 1} \qquad \text{...... (2.3)}$$

Left Hand Side of equation (2.2) and equation (2.3) represents Hypergeometric function.

But both of these equations have an undetermined element 'a' and 'b' which are needed to be determined to proceed further.

[3] Determination of 'a' and 'b'

To determine 'a' and 'b' for equation (2.2) and equation (2.3) respectively; we use the concept that [3], in Hypergeometric function $F(\alpha,\beta;\gamma;x)$, 'γ' is not negative and, 'α' and 'β' can be interchanged without affecting the value of $F(\alpha,\beta;\gamma;x)$.

As we are working here for the case of almost complete conversion; we will take,

$x_A = 1$

Then for $x_A = 1$, $F(\alpha,\beta;\gamma;x)$ converges when

$\gamma > \alpha + \beta$

And diverges when

$\gamma \le \alpha + \beta$

[I] Determination of 'a'

From equation (2.2) we have

$$F(n-1,a;a;x_A) \quad \left\{\tau_n k_n C_{A0}^{n-1}(n-1)\right\}+1 \qquad \text{...... (2.2)}$$

Case 1

If $F(n-1,a;a;x_A)$ is convergent. Then
$a > (n-1) + a$
$\Rightarrow n < 1$ ...... (3.1.1)
Also if (n-1) and 'a' are interchanged, then in this case it may be written as
$a = n - 1$ ...... (3.1.2)
Since in equation (2.2) we had
$\beta = \gamma = a$
So now we have,
$\beta \quad \gamma \quad n-1$
$\Rightarrow n-1 > 0$
$\Rightarrow n > 1$ ...... (3.1.3)

Equations (3.1.1) and equation (3.1.3) are contradictory in nature. Thus we discard this case and move to the next case.

Case 2

If $F(n-1,a;a;x_A)$ is divergent. Then
$a \le (n-1) + a$
$\Rightarrow n > 1$ ...... (3.1.4)
Also if (n-1) and 'a' are interchanged, then in this case it may be written as
$a = n - 1$ ...... (3.1.5)
Since in equation (2.2) we had
$\beta = \gamma = a$
So now we have,
$\beta \quad \gamma \quad n-1$
$\Rightarrow n-1 > 0$
$\Rightarrow n > 1$ ...... (3.1.6)
From equation (3.1.4) and equation (3.1.6) we get
$n > 1$
This also signifies three results:
(i) Equation (2.2) is to be used when $n > 1$
(ii) $a = n - 1$, in equation (2.2)
(iii) Series involved in equation (2.2) is divergent in nature.

[II] Determination of 'b'

From equation (2.3) we have

$$F(1-n,b;b;x_A) = \frac{1}{\left\{\tau_n k_n C_{A0}^{n-1}(n-1)\right\}+1} \qquad \text{...... (2.3)}$$

Case 1

If $F(1-n,b;b;x_A)$ is convergent. Then
$b > (1-n) + b$
$\Rightarrow n > 1$ ...... (3.2.1)
Also if $(1-n)$ and 'b' are interchanged, then in this case it may be written as
$b = (1-n)$ ...... (3.2.2)
Since in equation (2.3) we had

$\beta = \gamma = b$

So now we have

$\beta = \gamma = 1 - n$

$\Rightarrow 1 - n > 0$

$\Rightarrow n < 1$ …… (3.2.3)

Equations (3.2.1) and equation (3.2.3) are contradictory in nature. Thus we discard this case and move to the next case.

Case 2

If $F(1 - n, b; b; x_A)$ is divergent. Then

$b \leq (1 - n) + b$

$\Rightarrow n < 1$ …… (3.2.4)

Also if $(1 - n)$ and 'b' are interchanged, then in this case it may be written as

$b = (1 - n)$ …… (3.2.5)

Since in equation (2.3) we had

$\beta = \gamma = b$

So now we have

$\beta = \gamma = 1 - n$

$\Rightarrow 1 - n > 0$

$\Rightarrow n < 1$ …… (3.2.6)

From equation (3.2.4) and equation (3.2.6) we get

$n < 1$

This also signifies three results:

(i) Equation (2.3) is to be used when $n < 1$

(ii) $b = (1 - n)$, in equation (2.3)

(iii) Series involved in equation (2.3) is divergent in nature.

After determination of 'a' and 'b' we may proceed further with equation (2.2) and equation (2.3).

[4] Gauss's π-function for $x_A = 1$

When x is made unity in $F(\alpha, \beta; \gamma; x)$ it is denoted by $F_1(\alpha, \beta; \gamma)$ and its value is given in terms of Gauss's $\pi -$ function; given by A.R. Forsyth [3] as

$$F_1(\alpha, \beta; \gamma) = \left\{ \frac{\pi(\gamma - 1)\pi(\gamma - \alpha - \beta - 1)}{\pi(\gamma - \alpha - 1)\pi(\gamma - \beta - 1)} \right\} \quad \text{…… (4.1)}$$

[I] For $n > 1$

In this case, equation (2.2) has to be used

$$F(n - 1, a; a; x_A) = \left\{ \tau_n k_n C_{A0}{}^{n-1}(n - 1) \right\} + 1 \quad \text{…… (2.2)}$$

For $x_A = 1$, equation (2.2) becomes

$$F_1(n - 1, a; a) = \left\{ \tau_n k_n C_{A0}{}^{n-1}(n - 1) \right\} + 1 \quad \text{…… (4.2.1)}$$

Using result (4.1) and equation (3.1.5) in equation (4.2.1) we get

$$F_1(n - 1, a; a) = \left\{ \frac{\pi(n - 2)\pi(-n)}{\pi(-1)\pi(-1)} \right\} \quad \text{…… (4.2.2)}$$

Now we establish relationships between space times for two, different ordered reactions.

Consider the unimolecular type u^{th} ordered and v^{th} ordered two different reactions.

Here,

$u, v \in n$

$u > v$

$u - v = \delta$ …… (4.2.3)

For u^{th} ordered reaction, equation (4.2.2) becomes

$$F_1(u-1,a;a) = \left\{ \frac{\pi(u-2)\pi(-u)}{\pi(-1)\pi(-1)} \right\}$$

$$= \left\{ \tau_u k_u C_{A0}{}^{u-1}(u-1) \right\} + 1 \quad \text{…… (4.2.4)}$$

Similarly for v^{th} ordered reaction, equation (4.2.2) becomes

$$F_1(v-1,a;a) = \left\{ \frac{\pi(v-2)\pi(-v)}{\pi(-1)\pi(-1)} \right\}$$

$$= \left\{ \tau_v k_v C_{A0}{}^{v-1}(v-1) \right\} + 1 \quad \text{…… (4.2.5)}$$

Dividing equation (4.2.4) by equation (4.2.5)

$$\frac{\pi(u-2)\pi(-u)}{\pi(v-2)\pi(-v)} = \frac{\left\{ \tau_u k_u C_{A0}{}^{u-1}(u-1) \right\} + 1}{\left\{ \tau_v k_v C_{A0}{}^{v-1}(v-1) \right\} + 1} \quad \text{…… (4.2.6)}$$

Using equation (4.2.3) in equation (4.2.6) and generalizing in terms of Gamma function of Euler, we obtain

$$\left\{ \frac{\Gamma(u-1)\Gamma(-u+1)}{\Gamma(u-\delta-1)\Gamma(-u+\delta+1)} \right\} = \frac{\left\{ \tau_u k_u C_{A0}{}^{u-1}(u-1) \right\} + 1}{\left\{ \tau_v k_v C_{A0}{}^{v-1}(v-1) \right\} + 1} \quad \text{.... (4.2.7)}$$

Equation (4.2.7) is applicable for any real positive value of 'u' which is greater than unity.

Also in equation (4.2.7); 'δ' is always smaller than 'u'; which would not be the case when equation (4.2.6) is expressed in terms of 'v'. Thus, equation (4.2.7) is most generalized expression relating space times for two different ordered unimolecular reactions for order greater than unity.

[II] For $n < 1$

In this case, equation (2.3) has to be used

$$F(1-n,b;b;x_A) = \frac{1}{\left\{ \tau_n k_n C_{A0}{}^{n-1}(n-1) \right\} + 1} \quad \text{…… (2.3)}$$

For $x_A = 1$, equation (2.3) becomes

$$F_1(1-n,b;b) = \frac{1}{\left\{ \tau_n k_n C_{A0}{}^{n-1}(n-1) \right\} + 1} \quad \text{…… (4.3.1)}$$

Using result (4.1) and equation (3.2.5) in equation (4.3.1) we get

$$F_1(1-n,b;b) = \left\{ \frac{\pi(n-2)\pi(-n)}{\pi(-1)\pi(-1)} \right\} \quad \text{…… (4.3.2)}$$

Now we establish relationships between space times for two, different ordered reactions.

Consider the unimolecular type y^{th} ordered and w^{th} ordered two different reactions.

Here,

$y, w \in n$

$y > w$

$y - w = \varepsilon$ …… (4.3.3)

For y^{th} ordered reaction, equation (4.3.2) becomes

$$F_1(1-y,b;b)=\left\{\frac{\pi(y-2)\pi(-y)}{\pi(-1)\pi(-1)}\right\}$$

$$=\frac{1}{\left\{\tau_y k_y C_{A0}{}^{y-1}(y-1)\right\}+1} \quad \text{...... (4.3.4)}$$

Similarly for w^{th} ordered reaction, equation (4.3.2) becomes

$$F_1(1-w,b;b)=\left\{\frac{\pi(w-2)\pi(-w)}{\pi(-1)\pi(-1)}\right\}$$

$$=\frac{1}{\left\{\tau_w k_w C_{A0}{}^{w-1}(w-1)\right\}+1} \quad \text{...... (4.3.5)}$$

Dividing equation (4.3.4) by equation (4.3.5)

$$\frac{\pi(y-2)\pi(-y)}{\pi(w-2)\pi(-w)}=\frac{\left\{\tau_w k_w C_{A0}{}^{w-1}(w-1)\right\}+1}{\left\{\tau_y k_y C_{A0}{}^{y-1}(y-1)\right\}+1} \quad \text{...... (4.3.6)}$$

Using equation (4.3.3) in equation (4.3.6) and generalizing in terms of Gamma function of Euler, we obtain

$$\left\{\frac{\Gamma(y-1)\Gamma(-y+1)}{\Gamma(y-\varepsilon-1)\Gamma(-y+\varepsilon+1)}\right\}=\frac{\left\{\tau_w k_w C_{A0}{}^{w-1}(w-1)\right\}+1}{\left\{\tau_y k_y C_{A0}{}^{y-1}(y-1)\right\}+1} \quad \text{.... (4.3.7)}$$

Equation (4.3.7) is applicable for any real positive value of 'y' which is less than unity.

Also in equation (4.3.7); 'ε' is always smaller than 'y'; which would not be the case when equation (4.3.6) is expressed in terms of 'w'. Thus, equation (4.3.7) is the most generalized expression relating space times for two different ordered unimolecular reactions for order less than unity.

[5] Results and Conclusion

The relationships between space times for two different ordered reactions are thus dealt by equation (4.2.7) when $n>1$ and (4.3.7) when $n<1$.

By definition of gamma function we know that $\Gamma(z)$ has simple poles at
$z=0,-1,-2,-3,....$
and is non-analytic at these points.

In equation (4.2.7), a case may arise that 'u' and 'δ' simultaneously posses an integer value. This in turn gives rise to non-analyticity of gamma function.

Following two methods are preferred to deal with this situation.

[I] Weiestrass definition of Gamma Function

According to Weiestrass [4],

$$\frac{1}{\Gamma(z)}=ze^{\gamma z}\prod_{n=1}^{\infty}\left[\left(1+\frac{z}{n}\right)e^{\frac{-z}{n}}\right] \quad \text{...... (5.1.1)}$$

Where
γ = Euler's constant; defined as

$$\gamma \;\; \lim_{n\to\infty}\left(1+\frac{1}{2}+\frac{1}{3}+.....+\frac{1}{n}-\log_e n\right) \text{...... (5.1.2)}$$

From equation (5.1.1)

$$\Gamma(z) = \lim_{n\to\infty} \frac{(n!)n^{z}}{z(z+1)(z+2).......(z+n)} \quad ...... (5.1.3)$$

$$\Rightarrow \Gamma(z) = \lim_{n\to\infty} \int_0^n \left(1-\frac{t}{n}\right)^n t^{z-1}dt \quad ...... (5.1.4)$$

Equation (5.1.4) may be satisfactorily used to evaluate $\Gamma(z)$ very close to the simple poles.

In equation (5.1.4) if

$\mathrm{Re}(z) > 0$

Then it reduces to Euler's gamma function,

$$\Gamma(z) = \int_0^{\infty} e^{-t}t^{z-1}dt \quad ...... (5.1.5)$$

[II] Further Reduction of equation (4.2.7)

From equation (4.2.7) we have

$$\left\{\frac{\Gamma(u-1)\Gamma(-u+1)}{\Gamma(u-\delta-1)\Gamma(-u+\delta+1)}\right\} = \frac{\left\{\tau_u k_u {C_{A0}}^{u-1}(u-1)\right\}+1}{\left\{\tau_v k_v {C_{A0}}^{v-1}(v-1)\right\}+1} \quad .... (4.2.7)$$

As a special case, when u and v are positive integers greater than unity. The equation (4.2.7) can be reduced to,

$$\frac{\prod_{m=1}^{\delta}(u-1)-(m)}{\prod_{p=0}^{\delta-1}(-u+1)+(p)} = \frac{\left\{\tau_u k_u {C_{A0}}^{u-1}(u-1)\right\}+1}{\left\{\tau_v k_v {C_{A0}}^{v-1}(v-1)\right\}+1} \quad ..... (5.2.1)$$

Equation (5.2.1) also proves to be a valid tool to deal with this case.

In equation (4.3.7) no such case arises and it is most generalized form to deal with reactions with order less than unity.

[6] Further Discussions

$F(\alpha,\beta;\gamma;x)$ satisfies the differential equation

$$\frac{d^2w}{dx^2} + \left\{\frac{\gamma - x(1+\alpha+\beta)}{x(1-x)}\right\}\frac{dw}{dx} - \frac{\alpha\beta}{x(1-x)}w = 0 \quad ...... (6.1)$$

Equation (6.1) is called Hypergeometric Differential equation

At x=1; the function

$$P(x) = \left\{\frac{\gamma - x(1+\alpha+\beta)}{x(1-x)}\right\}$$

And

$$Q(x) = \left\{-\frac{\alpha\beta}{x(1-x)}\right\}$$

are both non- analytic.

Thus, x=1 is regular singular point of equation (6.1) with exponents;

0 and $\gamma-\alpha-\beta$.

So, we attempt to find the solution of equation (6.1) in neighborhood of x=1 by making the substitution $\xi = 1 - x$ in equation (6.1).

The solution comes out to be,

$$w = AF(\alpha,\beta;\alpha+\beta-\gamma+1;1-x)+B(1-x)^{\gamma-\alpha-\beta}F(\gamma-\alpha,\gamma-\beta;\gamma-\alpha-\beta+1;1-x)$$

…… (6.2)

Equation (6.2) is the linear combination of two solutions of equation (6.1)

Equation (6.2) can be used for further analysis of equation (2.2) and equation (2.3) for conversion very close to the complete conversion.

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