APPENDIX-3

RELATIONSHIP BETWEEN PARAMETERS AND TERMS APPEARING IN THE INTEGRAL EQUATIONS

During integral analysis, incorporation of the rate equation into the plug flow reactor equation followed by rearrangement leads to the following form,

$$\frac{W}{F_{Ao}} = \alpha \int_0^x \frac{dx}{(a+bx+cx^2)} + \beta \int_0^x \frac{dx}{(a+bx+cx^2)} + \gamma \int_0^x \frac{dx^2}{(a+bx+cx^2)}$$

The constants α, β, γ, a, b, c represent combinations of the parameters viz. reaction rate constant and adsorption equilibrium constants depending on the rate controlling step. Analytical solutions of these integrals yields the equation,

$$\frac{W}{F_{Ao}} = \frac{1}{C} (\alpha \tau_1 + \beta \tau_2 + \gamma \tau_3) \quad , \quad \text{where}$$

$$\tau_1 = \frac{1}{\sqrt{D}} \log \left| \frac{(2cx + b + \sqrt{D})(b + \sqrt{D})}{(2cx + b + \sqrt{D})(b - \sqrt{D})} \right|$$

$$\tau_2 = \frac{1}{2c} \left(\log \frac{a + bx + cx^2}{a} - b\tau_1 \right)$$

$$\tau_3 = \frac{1}{c} \left(x - \frac{b}{2c} \log \frac{a + bx + cx^2}{a} + \frac{b^2 - 2ac}{2c} \tau_1 \right)$$

$$D = b^2 - 4ac$$

The relationship of the constants α, β, γ, a, b, c with the parameters, viz. rate constant and adsorption constants for various models are tabulated below.

Model	C	α	β	γ
DSAC	k	$42K_H+49$	$14+6K_P+7K_O+13K_H$	$1+K_P+K_O+K_H$
DSSRC	kK_P	$49+7K_P+42K_H$	$2\sqrt{\alpha\cdot\gamma}$	$1-K_P+K_O+K_H$
DSODC	$kK_{eq}K_P$	$42+6K_P+7K_{eq}K_P+36K_H$	$13-5K_P-6K_{eq}K_P+12K_H$	$1+K_H-K_P-K_{eq}K_P$
DSHDC	$kK_{eq}K_P$	$42+6K_P+7K_{eq}K_P+36K_O$	$13-5K_P-6K_{eq}K_P+12K_O$	$1+K_O-K_P-K_{eq}K_P$
SSAC	k	49	$14+6K_P+7$	$1+K_P+K_O$
SSSRC	kK_P	$49+7K_P$	$14-6K_P+7K_O$	$1-K_P+K_O$
SSODC	$kK_{eq}K_P$	$42+6K_P+7K_PK_{eq}$	$13-5K_P-6K_PK_{eq}$	$1-K_P-K_{eq}K_P$
$a = -1-\frac{1}{K_{eq}}$, $b = -6-\frac{6}{K_{eq}}$ and $c = 7$ (a, b, c are common for all models)				

DSAC: Dual Site Adsorption Control

DSSRC: Dual Site Surface Reaction Control

DSODC: Dual Site Olefin Desorption Control

DSHDC: Dual Site Hydrogen Desorption Control

SSAC : Single Site Adsorption Control

SSSRC: Single Site Surface Reaction Control

SSODC: Single Site Olefin Desorption Control