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Hybrid Algorithm for Acceleration of Convergence to Cyclic Steady State

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Abstract: Cyclic process is inherently dynamic, thus it has no steady state. However, the process, after a sufficient number of cycles, will reach a state called Cyclic Steady State (CSS) where the process state variables at some instant within a cycle have the same value at the corresponding instant within each subsequent cycle. Depending on the nature of the cyclic process, the number of cycles needed before the process reaches CSS may vary from tens to thousands. In this study, a hybrid algorithm that aims to predict and accelerate the convergence of the CSS is developed and tested on a cyclic operation of controlled-cycled stirred tank reactor.

Key words: Hybrid algorithm, prediction of CSS, acceleration of CSS

INTRODUCTION

The nature of cyclic process has no steady state like general continuous process, it is inherently dynamic. Once the cyclic process is initiated, the process undergoes a transient stage prior to reach CSS. A cycle can be viewed as an orbit as shown in Fig. 1. With initial vector that composed of process states variables in the model equations, $\bar{X}_0$ the cycle transforms the initial vector to a new vector, $\bar{X}_n$ at the end of the cycle. When the new vector completely specifies the state of the bed at the beginning and end of the cycle, $\bar{X}_e$, CSS is reached and the process will repeatedly continue as a prefixed orbit (Croft and LeVan, 1994). At CSS, the process state variables at some instant within a cycle have the same value at the corresponding instant within each subsequent cycle (Choong *et al*., 2002).

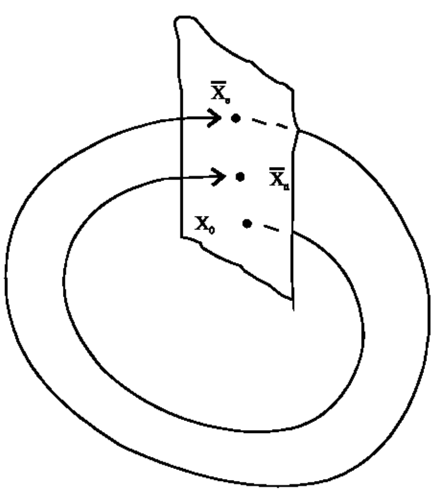

Fig. 1: Depiction of a cyclic process

MATERIALS AND METHODS

Controlled-Cycled Stirred Tank Reactor (CCSTR): The operation of the first cycle of a CCSTR is similar to a batch reactor. At the end of the first cycle, the mixture is not fully withdrawn but part of the mixture will remain in the reactor and mix with fresh feed for second cycle and so on (Razon, 2006). Figure 2 shows the operation of the

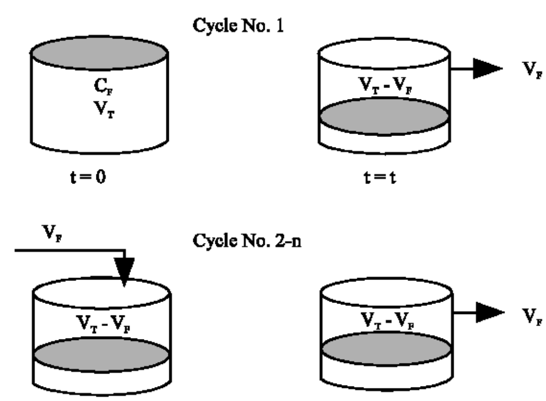

Fig. 2: Operation of CCSTR

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CCSTR. C_F is the concentration of the feed for each batch, V_F is the volume of reactant fed into each batch, V_T is the total volume of reactant and t is time.

The state variable for this operation is the conversion, $\bar{X}$. An implicit non-linear algebraic to solve for the n[th] batch conversion is given as:

$$\ln\left|\frac{f-\bar{X}_{n+1}}{f(1-\bar{X}_n)}\right| + K^*\left[\bar{X}_n - \frac{\bar{X}_{n+1}}{f}\right] + Da = 0 \quad (1)$$

where, K* is the multiplication of equilibrium constant and concentration of the feed of each cycle, f is the fraction of the reacting mixture removed at the end of cycle and Da is the Damkholer number.

The hybrid algorithm: The hybrid algorithm combines the Method of Successive Substitution (MSS) and the Aitken's updating formula. MSS is a direct substitution method whereby the results of previous cycle are used as the initial conditions for the next cycle. The Aitken's updating formula is a method of accelerating the rate of convergence where the new conversion, $\bar{X}_{new}$ can be estimated by:

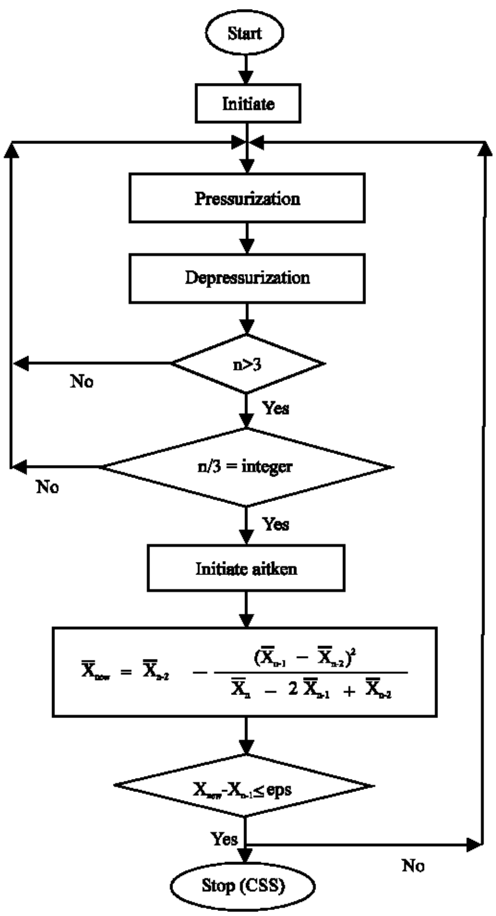

Fig. 3: Steps for the hybrid algorithm

Table 1: Comparison of results simulated by MSS and the hybrid algorithm

	MSS			Hybrid		
X_0	No. of cycle to CSS	X_{CSS}	Error (%)	No. of cycle to CSS	X_{CSS}	Error (%)
0.72	150	0.45008	0.00	120	0.45485	1.06
0.74	1374	0.45041	0.07	680	0.45016	0.02

$$\bar{X}_{new} = \bar{X}_{n-2} - \frac{(\bar{X}_{n-1} - \bar{X}_{n-2})^2}{\bar{X}_n - 2\bar{X}_{n-1} + \bar{X}_{n-2}} \quad (2)$$

To initiate, the Aitken's updating formula, the system is to be run for 3 cycles by MSS and the $\bar{X}_{new}$ will be then used as the initial condition to the next cycle. For every 3 subsequent MSS steps, Aitken will be initiated. When the difference between the Aitken's estimation of $\bar{X}_{new}$ and the X previous cycle, X_{n-1} is less than a small value, eps, the simulation will be terminated and CSS is reached. Steps of hybrid algorithm are shown in Fig. 3.

NUMERICAL SOLUTION

Equation 1 is solved numerically by using the Secant method, whereas the convergence of $\bar{X}_n$ is determined by using the hybrid algorithm. A tolerance of 1.0×10^{-9} for the Secant iteration is used and the iteration to the convergence of $\bar{X}_n$ is stopped when the eps is $\le 1.0\times10^{-9}$. Parameters used in the simulation are Da = 5.3069, K* = 8 and f = 0.5. The CSS reported by Razon (2006) under this condition is 0.45008.

The hybrid algorithm has showed reduction of number of cycles to reach CSS as compared to MSS. Table 1 shows a summary of tests using two initial conditions of 0.72 and 0.74.

CONCLUSION

The hybrid algorithm is shown to have the potential to reduce the number of cycle required to reach CSS for the CCSTR. More tests will be carried out on other cyclic processes.

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