HUNGARIAN JOURNAL
OF INDUSTRIAL CHEMISTRY
VESZPRÉM
Vol. 30. pp. 191 - 192 (2002)

MATHEMATICAL EQUIVALENCE OF INFINITE MIXED FLOW REACTORS IN SERIES AND PLUG FLOW REACTOR

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Received: December 30, 2001; Revised: July 8, 2002

This paper proves the mathematical equivalence of infinite mixed flow reactors in series and a plug flow reactor, in the time domain using an impulse input. The proof is mathematically less complicated, compared to the previous statements in the literature.

Keywords: chemical reactors, mixed flow reactor, plug flow reactor, residence time distribution, convergence

Introduction

The basic concept, that infinite mixed flow reactors (MFR) in series give the same performance as a plug flow reactor (PFR) is well known in chemical engineering for many years. But, only a few mathematical proofs of this concept are available in literature. Villermaux [1] proved the convergence in the Laplace domain. Molin and Gervais [2] showed the convergence in time domain with step input using limiting values of incomplete gamma function. Chen [3] used asymptotic equation for treatment of incomplete gamma function and proved the convergence in time domain with step input. In this work, the mathematical equivalence of a plug flow reactor and infinite mixed flow reactors in series is shown in time domain using an impulse input (Dirac delta function). The mathematical complexity is less, compared to the previous works.

Proof of Equivalence

A series of mixed flow reactors (MFRs) with delta input are shown in *Fig.1*. The dimensionless exit age distribution function, $E(\theta)$, for N tanks in series can be derived easily [4] as

$$E(\theta)=\frac{N(N\theta)^{N-1}e^{-N\theta}}{(N-1)!} \tag{1}$$

where $\theta = t/\tau$ is the dimensionless time, t is the time variable and τ the average residence time of the entire system. The response curves, *Eq.(1)*, for different number of MFRs in series (N = 1, 2, 5, 20, 50, 100, 200, 500 and ∞) are shown in *Fig.2*. As the number of tanks approaches infinity, the response approaches an impulse output with a time lag of average residence time τ (θ = 1) of the entire system. This response is characteristic of a plug flow reactor with delta input.

By definition of plug flow, each cross-section should correspond to an ideal mixer. Therefore intuitively a plug flow reactor can be considered as infinite mixed flow reactors in series. This is validated here mathematically, by proving that the function $E(\theta)$ tends towards a Dirac delta function with point of impulse at $\theta = 1$, as N tends towards ∞, which is the response of a plug flow reactor to an impulse input.

Using Stirling's approximation,

$$N!=N^{N}e^{-N}\sqrt{2\pi N} \tag{2}$$

and rearranging, *Eq.(1)* can be written as

$$E(\theta)=\frac{e^{(-N(-\ln\theta-1+\theta)-\ln\theta+(1/2)\ln N)}}{\sqrt{2\pi}} \tag{3}$$

To show that *Eq.(3)* approaches a Dirac delta function when N tends towards infinity, the following have to be proved [5]:

$$\begin{aligned} E(\theta) &= \infty \qquad & \theta = 1 \\ &= 0 \qquad & \theta \neq 1 \end{aligned} \tag{4a}$$

such that

$$\int_{-\infty}^{\infty} E(\theta)d\theta = 1 \tag{4b}$$

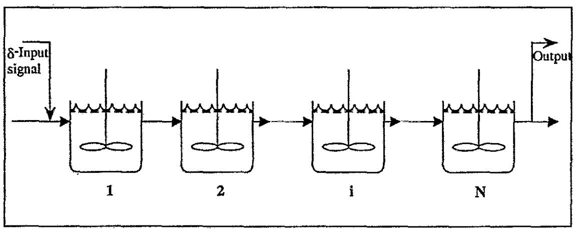

Fig.1 Schematic of MFRs in series

At $\theta = 1$, from *Eq.(3)*,

$$E(\theta) = \frac{\sqrt{N}}{\sqrt{2\pi}} \qquad (5)$$

Therefore as N approaches ∞, $E(\theta)$ tends towards ∞.

For values of θ in the intervals [0,1) and (1, ∞], $-\ln\theta -1+\theta$ is always positive. Therefore, the leading term in the exponent of *Eq.(3)* i.e. $-N(-\ln\theta -1+\theta)$ tends towards $-\infty$ as N approaches ∞. So in these intervals, $E(\theta)$ tends towards 0 as N tends to ∞.

Now, since negative values of θ are inadmissible,

$$\int_{-\infty}^{\infty} E(\theta)d\theta = \int_{0}^{\infty} E(\theta)d\theta = \frac{N^N}{(N-1)!}\int_{0}^{\infty} \theta^{N-1}e^{-N\theta}d\theta \qquad (6)$$

Using the definition of Gamma function [5],

$$\int_{0}^{\infty} \theta^{N-1}e^{-N\theta}d\theta = \frac{\Gamma(N)}{N^N} = \frac{(N-1)!}{N^N} \qquad (7)$$

Therefore, from *Eq.(6)*,

$$\int_{0}^{\infty} E(\theta)d\theta = 1 \qquad N \geq 1 \qquad (8)$$

Thus for infinite MFRs in series, the function $E(\theta)$ converges to a Dirac delta function characteristic of a plug flow reactor.

Conclusion

Using an impulse input, the equivalence of a series of infinite mixed flow reactors to a plug flow reactor is proved mathematically in the time domain. The proof is less complicated compared to the previous works in the literature.

SYMBOLS

$E(\theta)$ dimensionless exit age distribution function
N number of MFRs in series
t time variable, s

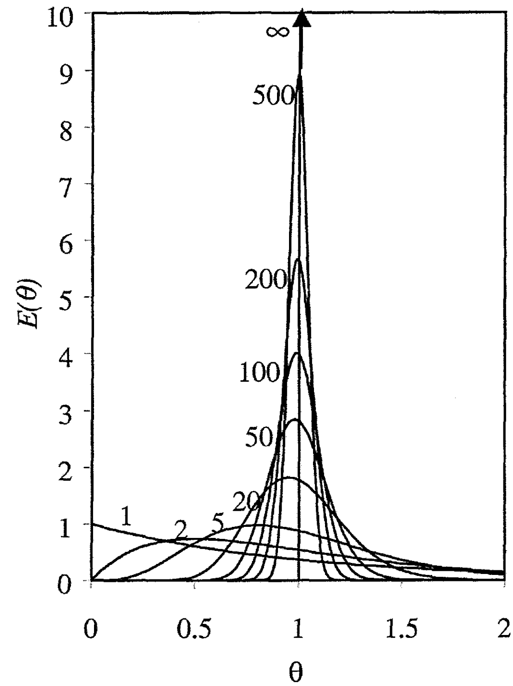

Fig.2 RTD curves for MFRs in series

Greek Letters

θ dimensionless time
τ average residence time, s
$\Gamma(N)$ Gamma function

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