This Week's Citation Classic®

Wehner J F & Wilhelm R H. Boundary conditions of flow reactor.
Chem. Eng. Sci. **6**:89-93, 1956.
[Department of Chemical Engineering, Princeton University, NJ]

An analysis is presented of the boundary conditions for a steady state flow-reactor with axial diffusion and first order reaction. Conclusions regarding reactor properties are reached as the result of simultaneous solution of the three differential equations for the reaction section and fore and after sections. Axial diffusion, but no reaction, may occur in the latter two sections. [The *SCI*® indicates that this paper has been cited in over 210 publications, making it one of the 10 most-cited papers published in this journal.]

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While spending a postdoctoral year at Princeton, I audited several graduate courses to help prepare myself to teach in chemical engineering, since my graduate work had been in chemistry. Among those courses was the kinetics and reactor design course taught by my coauthor, R.H. Wilhelm. The participants in this course were a talented group of first-year graduate students. While a paper by P.V. Danckwerts was being discussed, a question concerning the exit boundary conditions for a plug flow reactor was raised by a student. The answer was not apparent, and Wilhelm said that he would look for it. After class, I got into a discussion with him concerning the similarity between the entrance boundary condition and a problem in flame propagation that was the topic of my research project. He suggested the idea of a sectional reactor as described in the paper to study the boundary conditions. I agreed to look further into the idea and soon found that the mathematics was tractable, so we got together on a Saturday and wrote the paper. Since the results that we obtained included the results from Danckwerts's paper,[1] which had recently been published, we did not consider making a literature search.

It was quite disconcerting then to have it brought to our attention that Damköhler[2] had obtained a similar result years earlier using the identical technique that we used, and so we published an acknowledgement.[3] I learned only recently that Langmuir[4] had published a paper in 1908 that obtained Danckwerts's solution and was also overlooked by later authors. Nevertheless, publishing our paper at a time of increasing interest in theoretical work set off a great deal of activity that was further stimulated by Bischoff's results on more complex kinetics.[5]

A great many of the early citations to our paper were aimed at either extending the results or refuting them. In recent years, the citations have accepted the boundary conditions as a convenient starting point. Of much interest is Deckwer and Mählmann's work on the verification of the proper boundary conditions by considering reactors with more than three sections.[6] They also have performed careful experimental work investigating the jump conditions that arise in the absence of diffusion. They found a jump instead of the continuity I favored, although I would prefer to see more measurements before accepting the jump completely.

1 **Danckwerts P V.** Continuous flow systems distribution of residence times. *Chem Eng Sci* 2 1-13, 1953
[See also **Danckwerts P V.** Citation Classic. *Current Contents/Engineering Technology & Applied Sciences* 10(19) 16, 7 May 1979.]
2 **Damköhler G.** Einflusse der Strömung, Diffusion und des Wärmeüberganges auf die Leistung von Reaktionsöfen II. Die isotherme, raumbeständige homogene Reaktion erster Ordnung. *Z Elektrochem* 43 1-13, 1937
3 **Wehner J F & Wilhelm R H.** Note in connexion with the paper "Boundary conditions of flow reactor." *Chem Eng Sci* 8 309, 1958
4 **Langmuir I.** The velocity of reactions in gases moving through heated vessels and the effect of convection and diffusion. *J Amer Chem Soc* 30 1742-54, 1908.
5 **Bischoff K G.** A note on boundary conditions for flow reactors. *Chem Eng Sci* 46 131-3, 1961
6 **Deckwer W D & Mählmann E A.** Boundary conditions of liquid phase reactors with axial dispersion. *Chem Eng J* 11 19-25, 1976

