



TOGETHER
for a sustainable future

OCCASION

This publication has been made available to the public on the occasion of the 50th anniversary of the United Nations Industrial Development Organisation.



TOGETHER
for a sustainable future

DISCLAIMER

This document has been produced without formal United Nations editing. The designations employed and the presentation of the material in this document do not imply the expression of any opinion whatsoever on the part of the Secretariat of the United Nations Industrial Development Organization (UNIDO) concerning the legal status of any country, territory, city or area or of its authorities, or concerning the delimitation of its frontiers or boundaries, or its economic system or degree of development. Designations such as “developed”, “industrialized” and “developing” are intended for statistical convenience and do not necessarily express a judgment about the stage reached by a particular country or area in the development process. Mention of firm names or commercial products does not constitute an endorsement by UNIDO.

FAIR USE POLICY

Any part of this publication may be quoted and referenced for educational and research purposes without additional permission from UNIDO. However, those who make use of quoting and referencing this publication are requested to follow the Fair Use Policy of giving due credit to UNIDO.

CONTACT

Please contact publications@unido.org for further information concerning UNIDO publications.

For more information about UNIDO, please visit us at www.unido.org

16952

Distr.
LIMITED
IPCT.69(SPEC.)
11 July 1988
ORIGINAL: ENGLISH

UNITED NATIONS
INDUSTRIAL DEVELOPMENT ORGANIZATION

PHTHALIC AND MALEIC ANHYDRIDE SYNTHESSES*

Prepared by

José Luis Herce Vigil**

A. Hale***

- 166
-
- * This document has been reproduced without formal editing.
 - ** Universidad Autónoma Metropolitana, Av. San Pablo 180, Azcapotzalco, 02200 México 16, D.F.
 - *** University of Minnesota, Minneapolis, MN 55455, USA.

INTRODUCTION

The subject of this report is the selective oxidation of o-xylene and benzene and is a further contribution towards establishing the interest of considering the influence of adequate kinetic systems and mathematical models, the effect of catalyst ring stacking in the tube bundles of catalytic reactors and the influence of a non-boiling cooling flow when studying and operating exothermal tubular catalytic reactors. Some of the various kinetic equations in the available literature were considered in order to define steady state kinetic of the oxidation reactions in fixed bed reactors. Uni- and bi-dimensional model reactors were taken in account for the catalytic pilot reactor simulations to calculate temperature and concentration profiles. The rings coated with a catalyst ($V_2O_5 + TiO_2$) were placed in the tube bundle randomly, aligned (coaxial stacking with the cylindrical axis vertical) and shifted (with the cylindrical axis vertical). Recent studies have indicated that the influence of the cooling flow should be considered in detail for both the design and operation of multitubular catalytic fixed bed reactors. In fact, some contributions (1,2) have shown the key importance of the thermal changes in the cooling medium when modelling catalytic fixed bed reactors and when predicting "hot spots". The coolant, usually a molten salt in modern orthoxylene oxidation plants (3-6) gains sensible heat during its circulation (no phase change would be involved) and increases temperature significantly. This heat when removed from the reactor can be transferred to an external boiler (4,6). This aspect of the thermal behaviour of the cooling medium differs from a constant coolant temperature condition frequently adopted (7,8) and is only suitable for catalytic multitubular reactors employing a boiling liquid or a liquid of an abnormally large heat capacity as its cooling medium. These facts provide the reason to believe that when modelling orthoxylene oxidation reactors the thermal gradients in the fused salt side of the reactor must be considered as well as the interactions of those gradients on the temperature profiles inside the catalytic beds. As a consequence, complex instrumentation was installed to sense conventional "hot spots" located at unknown points between the reactor entry and reactor exit. This "hot spot" sensing problem becomes extremely critical in orthoxylene and benzene oxidation multitubular reactors when a non-boiling coolant is circulated under crossflow pattern (1).

It was also possible to analyse gas compositions along the reactor to determine conversion and concentration along the tube. These experimental data, together with heat reaction data and some of the various kinetic equations to be found in the literature were considered in the study for an appropriate description and simulation of the orthoxylene and benzene oxidation in pilot scale units.

The studies were carried out on a fixed bed pilot reactor (3m) with industrial non-porous vanadium-type catalysts.

KINETICS OF THE CATALYTIC ORTHOXYLENE AND BENZENE OXIDATION

When proceeding to the review of the different kinetic models and their significance in the context of the present study it was realized that the key element for the selection of a particular model was the observed phthalic anhydride yields. For instance, it may be noticed in Table 1 that V_2O_5 supported on SiC or TiO_2 give high phthalic anhydride yields, normally ranging between 70-85% (9-12). Conversely, V_2O_5 supported on SiO_2 gives

pure phthalic anhydride yields 15-45% (13,14). Consequently, the models referred to as 1 to 4 (Table 1) corresponding to catalysts giving a high phthalic anhydride yield, were considered as the basis for the formulations of the catalytic tubular reactor. It is important to mention at the same time that the kinetic models reported in Table 1 contain different specifications concerning the chemical network:

- intermediate products (o-tolualdehyde, phthalide and maleic anhydride)
- the CO/CO₂ product ratio (x value in CO_x formula).

Finally, the four kinetic models selected for those simulations consider an important characteristic of the catalytic orthoxylene oxidation process: the phthalic anhydride can be a final product or an intermediate chemical to be subsequently converted into carbon oxides. These two possible behaviours with respect to the phthalic anhydride led to different results. For the case of the catalytic oxidation of benzene, the most generally accepted reaction scheme was considered as valid.(15-18)

MATHEMATICAL MODEL

The highly exothermic complex reaction systems with several products are very complicated to simulate due to the enormous heat production that induces strong temperature gradients in both axial and radial directions. The models were extremely sensitive to thermal parameters and the simple models could be easily eliminated.

The oxidation of benzene and o-xylene are highly exothermic reactions that produce important temperature gradients. Permanent deactivation of the catalyst in such cases can be avoided only if the temperature profile is known. For these reasons it can be assumed that the fundamental equations should include axial and radial terms.

Previous works have demonstrated that temperature concentration gradients between particles and fluid and inside the particles themselves cannot be neglected. The evaluation of heat and mass transfer parameters in the interface particle-fluid and in the particle is not simple. In the case of maleic and phthalic anhydride syntheses the problem is simplified by the fact that the new catalysts are produced in a non-porous support, that is, the catalyst is located only as a thin layer over the external surface of the support. Therefore pore-diffusion does not have to be considered.

Pseudo-homogeneous uni- and bi-dimensional models were considered for the tubular catalytic fixed bed reactor simulations. These models are based on the following:

- Mass and thermal axial dispersion effects may be neglected. This seems a reasonable approximation considering a high axial Peclet number and that the relationship between reactor length and particle diameter is sufficiently high as can be evaluated from Table 2. This axial Peclet number is several times the critical value below which the axial dispersion effects become significant (19-21). In the present paper the authors verified this assumption during the simulation and as a consequence it was possible to adopt the piston flow model.

- Thermal and concentration differences between the catalyst particle and the fluid may be neglected. These same assumptions were considered in previous papers (22-24) and were reconfirmed by traditional calculations when estimating such gradients (25). These latter simplifications are also confirmed by the observed constancy of the energies of activation in the 623-715°K range (9,10,26,27). However, in the case of the active V₂O₅ supported on TiO₂ of model 4, it was more difficult to assess the possibilities of potential intraparticle diffusional limitations (1,28). The condition of chemical reaction control for this temperature range was then also assumed to be valid in order to illustrate the behaviour of this catalyst.
- The partial pressure of oxygen in the reactor remains essentially unchanged and equal to the initial oxygen concentration.
- Density and heat capacity parameters are assumed to be independent of temperature for the range of operating conditions considered in this study. The possible influence of the variation of these parameters with the temperature was also evaluated. Its influence on the temperature and concentration profiles was found negligible (27).
- Negligible pressure drop in the bed may be assumed for the calculations. This is a reasonable approximation, taking into account the 3-17 kPa pressure drop values that may be predicted in a 2-3m fixed bed containing cylindrical particles.

Taking into consideration the previous assumptions, the equations describing the heat and mass balances in the reactor tubes may be derived. The numerical solution of equations (1) and (2) permits the description of the concentration and temperature changes with the axial and radial reactor position. In fact, because of the cocurrent circulation of reactants and a non-boiling coolant, both profiles develop symmetrically and a single tube simulation would provide the required information for estimating the unit performance. Radial gradients in the cooling fluid were measured. It was found that they could be neglected.

EXPERIMENTAL

Apparatus

Using two flowmeters, streams of dried air and o-xylene (or benzene) were measured and combined to form a mixture containing about 1% of this compound. The mixture was preheated and then introduced into the reactor containing a V₂O₅ industrial catalyst (Figure 1). Operational characteristics are summarized in Table 2.

The rings of catalyst were placed in the reactor tube in three different forms: randomly, aligned and shifted.

Analysis

Gas compositions of feed, reactor and product currents were analysed (that is maleic and phthalic anhydrides, phthalide, tolual-aldehyde, etc.) by flame gas chromatography (Varian 1400). Inorganic compounds were analysed by a thermal conductivity chromatograph (VARIAN 1520) after eliminating water and organic compounds through coal and silica gel traps (30). Both chromatographs were connected to an electronic integrator in order to determine the concentration profiles (Figure 2).

NUMERICAL METHOD

One of the problems of this work was to find the values of the activation energies and the effective thermal conductivity which, when used in the simulation programme, would yield a temperature profile as similar as possible to the measure profile. This problem was approached as an optimization case. The objective function is the minimization of the discrete sum of the absolute values of the differences between computed and measured temperatures.

The optimization algorithm employed was the sequential simplex. This algorithm can be explained as follows: let us assume that a function $f(X_1, X_2)$ is to be optimized. The first step is to evaluate the function at three points (X_{11}, X_{21}) , (X_{12}, X_{22}) , (X_{13}, X_{23}) which should be equidistant from each other, thus forming an equilateral triangle. The point at which f has the worst value is then rejected and replaced by a point obtained by reflecting the rejected point in the opposite side of the original triangle. This new point together with the two remaining points form a new equilateral triangle. The procedure is then repeated until the value of f begins to cycle without further improvement. According to the wanted degree of precision, the procedure can be stopped at this point or can be repeated but with smaller distances between the points.

Sometimes a newly calculated point may happen to be the same which has been rejected in the prior iteration. In that case the second worst value of f should be rejected in order to avoid an endless loop.

This procedure can be easily expanded to n -dimensions. To obtain the co-ordinates of the starting points, the following formula is used:

$$X_{ij} = X_{i1} + d_{ij}$$

where X_{i1} is the i th co-ordinate of a base point 1, and d_{ij} is obtained from the following table:

Point j	d_{1j}	d_{2j}	d_{3j}	... d_{n-1j}	d_{nj}
1	0	0	0	0	0
2	p	p	q	q	q
3	q	q	q	q	q
.
.
.
n	q	q	q	p	q
n+1	q	q	q	q	p

where

$$p = (a/n \sqrt{2})(\sqrt{n+1} - n-1)$$

$$q = (a/n \sqrt{2})(\sqrt{n+1} - 1)$$

where a is the distance between any two points j and k

$$a^2 = \sum (X_{ij} - X_{ik})$$

Current anhydride production processes could be optimized in several ways: by increasing the number of tubes, the concentration of reactives at the entrance and the feed and improving the selectivity of the catalyst.

- The number of tubes in the multitubular reactor is normally limited to 20,000. There is another possibility of increasing the production capacity which involves the division of the reactor into two sections which are kept at different operating temperatures. In traditional fixed bed reactors the temperature near the reactor entrance is too high and the temperature in the reactor tail too low to achieve the optimal combination of conversion and selectivity which results in maximum yield. This problem can be avoided, however, if the reactor is divided into two sections with the first section being cooled to a considerably lower temperature than the second section, but here it is necessary to consider two questions: which are the optimal temperatures in the two sections and at which point should the reactor be divided in order to achieve the maximum yield. Some authors have studied this possible solution (31).
- A higher reactive concentration at the entrance could reach the explosion value of the reactive mixture and higher temperatures are to be obtained as a consequence of higher reaction rates.
- A higher volumetric feed will increase the pressure drop in the packed tubes. The pressure drop increases approximately in a quadratic way with the velocity of the gaseous mixture and in a linear way with the length of the tubes. It could reach higher values according to the form and size of the pellets.
- The selectivity of the catalyst could be improved in a certain extent (24), its life time could be extended and the limited heat transfer restricting selectivity could be increased. All three shortcomings depend on the temperature distribution in the reactor. The development of temperature hot spots has a detrimental effect on reactor yield and catalyst life time. If these hot spots could be avoided altogether and the reaction could be run in an isothermal reactor, yield and catalyst life time could be improved. Alternative reactor technologies are being developed for the future but the only immediate alternative is to find ways to lower the temperature hot spot and to approach the isothermal reactor through practical measures that can be implemented directly in industrial operations. A new approach to achieve this goal was considered in this work: the use of catalyst pellets of the same shape and heat transfer characteristics in the reactor but bundlessly stacked in the tube.

An increase in the volumetric feed results in an improvement of mass and heat transfer in the system but also in the pressure drop. In order to maintain it into reasonable values, different forms and stacking of catalysts are frequently discussed. Experiments were done for three different arrangements of the catalysts: randomly, aligned and staggered. Pressure drop in the arranged catalyst bed was considerably lower, specially for the case of an aligned catalyst whose value is only a fourth of the case of random arrangement. This is of special interest because of the void space in the reactor which goes down from 69 to 64%.

Axial temperature profiles for the different arrangements of the catalyst are shown in Figure 5 for an average volumetric feed of $2 \text{ m}^3/\text{h}$. The use of an aligned catalytical bed shows the highest increase in the hot spot region of the reactor. The staggered arrangement produces the lowest hot spot. In these two cases the greater amount of catalyst in the reactor has also to be taken into consideration. Another interesting feature is the radial heat transfer which is also affected, while higher gradients are produced as a possible consequence of channeling. Figure 6 shows such radial temperature differences.

Concentration profiles (Figure 7) are also different. More important turbulence in the staggered bed could be expected compared to the aligned one and as a result its concentration profile should be closer to the random bed concentration profile. Nevertheless, turbulence is not the only factor affecting the profile, a higher temperature in the first part of the reactor for the aligned bed produces a higher reaction rate. This higher rate, associated with a higher bed density is predominant. Its influence seems to be more important than the improvement in the mass transfer coefficient produced by the staggered catalyst.

Figure 8 shows the influence of volumetric feed over the different beds for constant initial o-xylene concentration. Volumetric feed did not have an important influence over conversion and yield until values of $2 \text{ m}^3/\text{h}$ were achieved. The yield was a slightly smaller in the case of the aligned bed, possibly as a consequence of higher temperatures. A volumetric feed of $3 \text{ m}^3/\text{h}$ produced important changes in yield and conversion.

Lower temperatures were obtained in the case of a staggered catalyst and these produced lower conversion and yield, thereby increasing sub-products amounts. This situation can be observed in Figure 7.

In Figure 8 we included the production of phthalic anhydride per unit of time and reactor volume. For the aligned bed the highest value was obtained with a volumetric feed of $3 \text{ m}^3/\text{h}$, 25% higher than in the case of the random bed. The pressure drop was about a fourth of that obtained with a non-arranged bed. The highest value for the shifted bed was obtained with a volumetric feed of $2 \text{ m}^3/\text{h}$ but it is inferior to that obtained in the aligned bed with $3 \text{ m}^3/\text{h}$, possibly as a consequence of lower temperatures.

CONCLUSION

It could be concluded that there was a necessity for:

- the use of two-dimensional reactor models in order to achieve a better simulation of the reactor;
- the adequacy of Calderbank models to represent the kinetics of ortho-xylene oxidation and of the simple model to represent the kinetics of benzene oxidation;
- the importance of knowing the thermal changes in the cooling medium;
- the advantages of catalyst ring stacking in the tube of a catalytic reactor.

With lower pressure drops produced through catalyst ring stacking, it is possible to use higher volumetric feeds and to increase the production of phthalic anhydride per unit of reactor volume. The utilization of longer reactors may also be possible.

REFERENCES

1. de Lasa, H.I., Mok, L.K., Soria Lopez, A., Oxidation of Ortho-xylene in a Catalytic Packed Bed Reactor. The Cross Flow Operation. The Critical Row of Tubes, Proceeding Second World Chem. Engng. Conf., 31st CSE Meeting, Montreal, Vol. III, 297 (1981)
2. Soria López, A., de Lasa, H., Porras, J.A., Parametric Sensitivity of a Fixed Bed Catalytic Reactor. Cooling Fluid Flow Influence, Chem. Eng. Sci. 36, 285-291 (1981)
3. Pinchbeck, P.H., Markham, H., The Fluidized Bed Process for the Manufacture of Phthalic Anhydride, I. Chem. E. Symp. Series (Inst. Chem. Engrs. London) 27, 189-194 (1968)
4. Froment, G.F., Fixed Bed Catalytic Reactors. Technological and Fundamental Design Aspects, Chemie-Ing. Techn. 46, 374-387 (1974)
5. Rase, H., Chemical Reactor Design for Process Plants. Vol. II, 123-131, J. Wiley, New York (1977)
6. Spitz, B.H., Phthalic Anhydride Revisited, Hydrocarbon Process, 47, 11, 162-168 (1968)
7. Hlavacek, V., Packed Catalytic Reactors, Ind. Eng. Chem. 62, (7), 8-26 (1970)
8. Froment, G.F., Fixed Bed Catalytic Reactors, Ind. Eng. Chem. 59, (2), 18-27 (1967)
9. Calderbank, P., Kinetics and Yields in the Catalytic Oxidation of O-Xylene to Phthalic Anhydride with V_2O_5 Catalysts, Adv. Chem. Series, 133, 646-653 (1974)
10. Calderbank, P.H., Chandrasekharan, K., Fumagalli, C., The Prediction of the Performance of Packed Bed Catalytic Reactors in the Air Oxidation of O-Xylene, Chem. Eng., Sci, 32, 1435-1443 (1977)
11. Wainwright, M.S., Hoffman, T.W., The Oxidation of O-Xylene in a Transported Bed Reactor, Adv. Chem. Series 133, 669-685 (1974)
12. Chandrasekharan, K., Calderbank, P.H., Prediction of Packed Bed Catalytic Reactor Performance for a Complex Reaction (Oxidation of O-Xylene to Phthalic Anhydride), Chem. Eng. Sci., 34, 1323-1331 (1979)
13. Boag, I.F., Bacon, D.W., Downie, J., Analysis of the Reaction Network for the Vanadia Catalyzed Oxidation of Ortho-xylene. J. Catal. 38, 375-384 (1975)
14. Wainwright, M.S., Hoffman, T.W., The Oxidation of Ortho-xylene on Vanadium Pentoxide Catalyst II. The Influence of Catalyst Support Material on Product Distribution, Can. J. Chem. Eng. 55, 557-564 (1977)
15. Phung Quach, T.Q., Rouleau, C., Chavarie, C., Laguerie, C., Catalytic Oxidation of Benzene to Maleic Anhydride in a Continuous Stirred Tank Reactor, Can. J. Chem. Eng. 56, 72078 (1978)
16. Dmuchovsky, M. Freerks, Pierron, F., Munch, R., Zienty, F., J. Catal. 4, 291 (1965)
17. Emmett, P.H., Catal. 7, 185 (1960)
18. Vaidynathane, K., Doraiswamy, L.K., Chem. Eng. Sci, 23, 537 (1968)
19. Froment, G.F., Analysis and Design of Packed Bed Catalytic Reactors, Adv. Chem. Series, 109, 1-34 (1972)
20. Froment, G.F., Bischoff, K.B., Chemical Reactor Analysis and Design, J. Wiley, New York (1979)
21. Carberry, J.J., Wendel, M.W., A Computer Model of the Fixed Bed Catalytic Reactor, AIChE J., 9, 129-133 (1963)
22. Herce-Vigil, J.L., Hale, A., Bugarel, R., Reaction Engineering of Anhydride Synthesis, Proceedings Third World Congress of Chem. Eng. Paper 9a-308, 152-155, Tokio (1986)

23. Herce-Vigil, J.L., Boehning, K., Luft, G., Análisis de las Variables de Diseño de Reactores para la Fabricación de Anhídrido Ftálico, Revista del Inst. Mex. de Ing. Quím. 1, 36-43 (1983)
24. Herce-Vigil, J.L., Flores J., Fraczak, M., Bugarel, R., Selective Catalyst for Some Anhydride Synthetis, 8 ICC, V-509-518 (1984)
25. Smith, J.M., Chemical Eng. Kineics, 3rd Ed., Chap. 9, McGraw-Hill, New York (1980)
26. Calderbank, P.H., Watt, G.J., Ellis, S.N., Some Aspects of the Strategy of Phthalic Anhydride Production by the Catalytic Oxidation of O-Xylene, Proceedings Fifth European Symp. Chem. Reaction Eng., Elsevier Amsterdam, Paper B2, 1-7 (1972)
27. Herce-Vigil, J.L., Hale, A., Cinética y Simulación de Ractores. Aplicación a la Síntesis de Anhídrido Ftálico, Programas de Computación en Ing. Química, COSNET, 39-71, México (1984)
28. Wainwright, M.S., Hoffman, T.W., The Oxidation of Orthoxylene on Vanadium Pentoxide Catalysts I. Transient Kinetic Measurements, Can. J. Chem. Eng. 55, 552-556 (1977)
29. Wainwright, M.S., Hoffman, T.W., The Oxidation of Ortho-xylene on Vanadium Pentoxide Catalysts II. The Influence of Catalyst Support Material on Product Distribution, Can. J. Chem. Eng. 55, 557-564 (1977)
30. Boehning, K.H., Diplomarbeit, T.H. Darmstadt, FRG (1981)
31. Wellaver, T.P., Cresswell, D.L., Newson, E.J., Optimal Policies in Maleic Anhydride Production Through Detailed Reactor Modelling, Chem. Eng. Sci. 41, 4, 765-772 (1986)
32. de Lasa, H., Application of the Pseudoadiabatic Operation to Catalytic Fixed Bed Reactors, Canad. Journal of Chem. Eng. 61, 710-718 (1983)

Table 1: Catalytic Orthoxylene Oxidation Reaction Networks

Model	Reference	Catalyst	T_{range} (K)	PA Yields P_B/P_A
o-xylene $\left\{ \begin{array}{l} \text{PA} \\ \text{CO} + \text{CO}_2 + \text{H}_2\text{O} \end{array} \right.$	(9, 26)	Promoted V_2O_5 on SiC	643-727	0.58-0.62 0.6-0.648
o-xylene $\left\{ \begin{array}{l} \text{PA} \\ \text{CO} + \text{CO}_2 + \text{H}_2\text{O} \end{array} \right.$	(8)	V_2O_5 on an unknown support	628-693	0.70-0.72
o-xylene - intermed. - $\left\{ \begin{array}{l} \text{PA} \\ \text{CO} + \text{CO}_2 + \text{H}_2\text{O} \end{array} \right.$	(10)	Unpromoted V_2O_5 on SiC	645-869	0.72-0.75
o-xylene - intermed. - $\left\{ \begin{array}{l} \text{PA} \\ \text{CO} + \text{CO}_2 + \text{H}_2\text{O} \end{array} \right.$	(29)	Promoted V_2O_5 on TiO_2	625-675	0.80-0.85
Benzene - MA $\left\{ \begin{array}{l} \text{MA} \\ \text{CO} + \text{CO}_2 + \text{H}_2\text{O} \end{array} \right.$	(15-18)	V_2O_5 on SiO_2	553-703	0.65-0.70

$$\epsilon D_{cr} \left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) - u_s \frac{\partial c}{\partial z} - r_{APB} = 0 \quad (1)$$

$$\lambda_{cr} \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) - u_s \rho c_p \frac{\partial T}{\partial z} + (-\Delta H) r_{APB} = 0 \quad (2)$$

with B.C. $c = c_0$ and $T = T_0$ at $z = 0$ for $0 < r < R_t$,
 $\partial c / \partial r = 0$ at $r = 0$ and $r = R_t$ for all z ,
 $\partial T / \partial r = 0$ at $r = 0$,
 $\partial T / \partial r = -(\alpha_w / \lambda_{cr})(T_R - T_w)$ at $r = R_t$.

Table 2 Reactor and Catalysts Characteristics

	o-Xylene system	Benzene system	
feed	0.5 - 4	2.2 - 5	m ³ h ⁻¹
o-xylene	0.35 - 1	0.5 - 1	% mol
air	99 - 99.5	99 - 99.5	% mol
pressure	1	1	atm
feed temperature	350 - 356	350 - 365	C
cooling system	350 - 385	350 - 385	C
reactor length	3	3	m
reactor diameter	0.025	0.025	m
catalyst	V ₂ O ₅ - K ₂ SO ₄	V ₂ O ₅ - MoO ₃	
form	rings	rings	
length	7 x 10 ⁻³	7 x 10 ⁻³	m
diameter	7 x 10 ⁻³	7 x 10 ⁻³	m
wall thickness	1.5 x 10 ⁻³	1.5 x 10 ⁻³	m
density	1.87 x 10 ³	1.68 x 10 ³	Kg m ⁻³
bed density	1.05 x 10 ³	1.166 x 10 ³	Kg m ⁻³
bed porosity	0.56	0.34	

NOTATION

c	concentration of reference component in the fluid (kmol/m ³)
c ₀	inlet concentration (kmol/m ³)
c _p	specific heat (kcal/kg K)
D _{er}	effective diffusivity in radial direction (m ² /m h)
ΔH	heat of reaction (kcal/kmol)
r _A	rate of reaction based on component A (kmol/kg cat h)
r	radial coordinate
R _t	tube radius (m)
T	fluid temperature (K)
T _R	bed temperature at radius R _t (K)
T ₀	inlet fluid temperature (K)
T _w	wall temperature (K)
u _s	superficial velocity (m ³ /m ² h)
z	axial coordinate
α _w	wall heat transfer coefficient (kcal/m ² h K)
ε	void fraction of the bed
λ _r	effective thermal conductivity in radial direction (kcal/m h K)
ρ _f	fluid density (kg/m ³)
ρ _B	catalyst bulk density (kg cat/m ³)

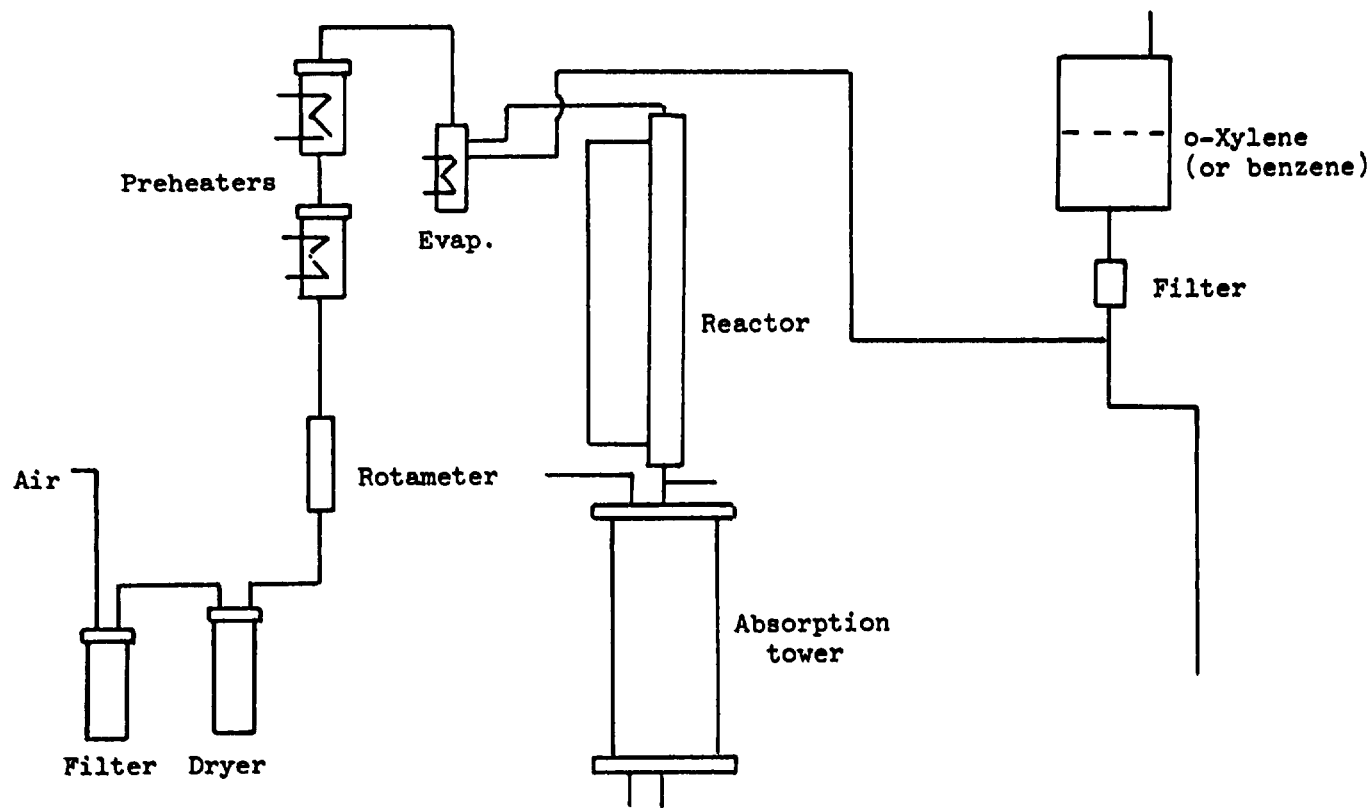


Fig. 1 Apparatus

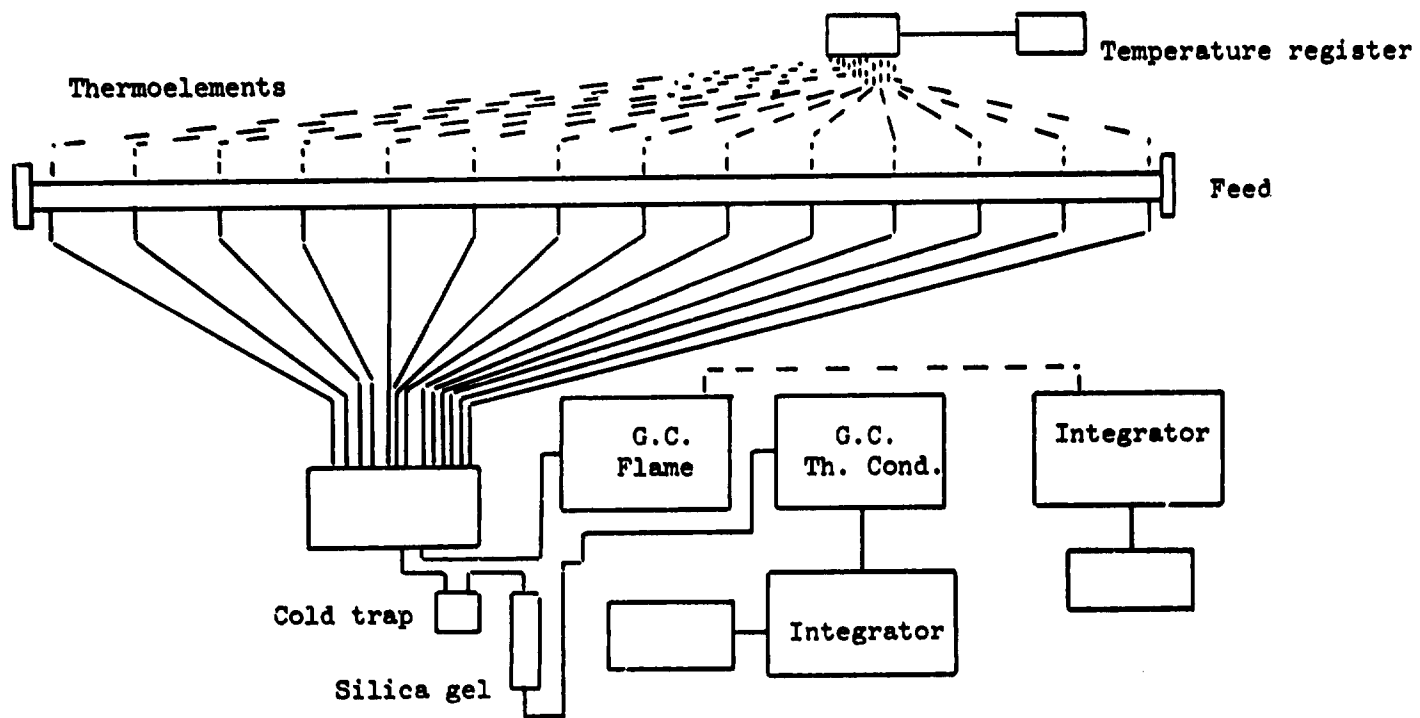


Fig. 2 Analysis system

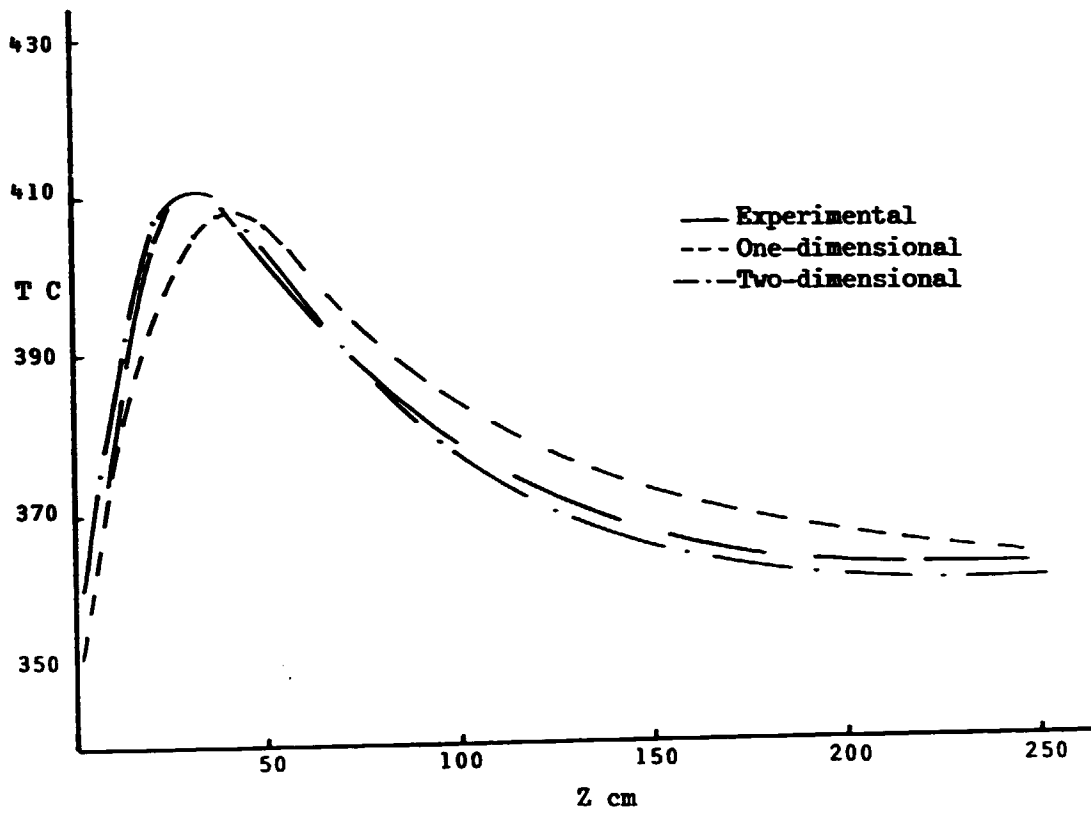


Fig. 3 Temperature profile

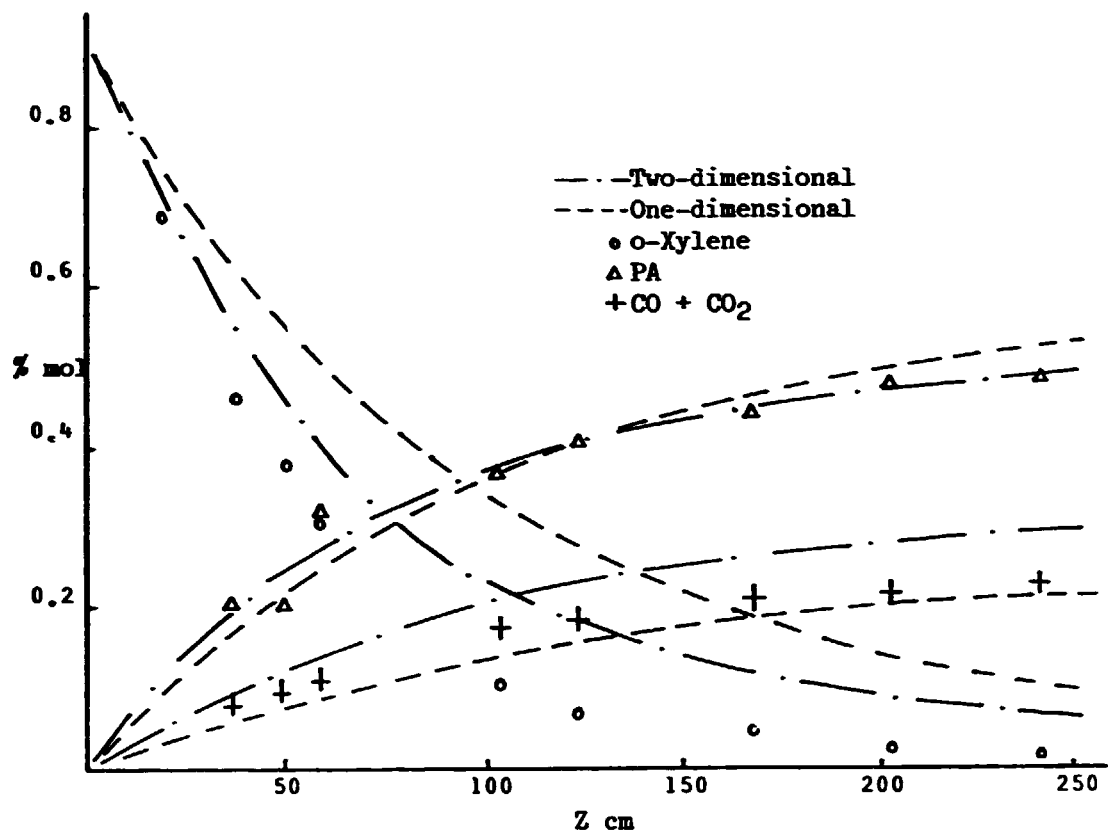


Fig. 4 Concentration profile

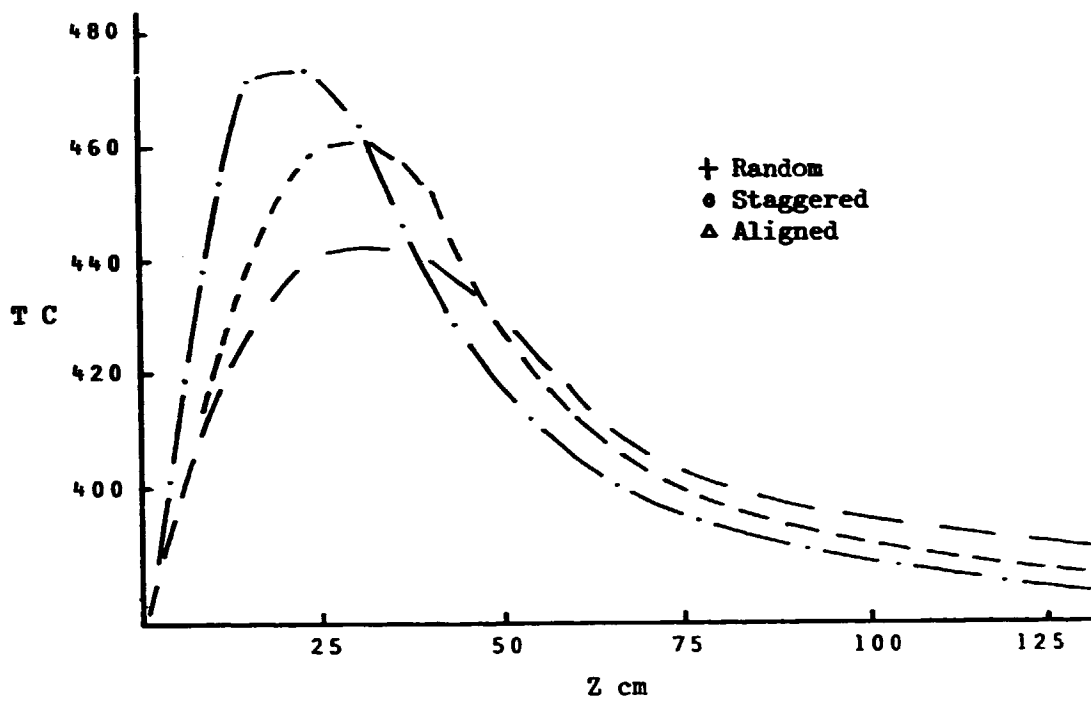


Fig. 5 Axial temperature profiles for the different arrangements

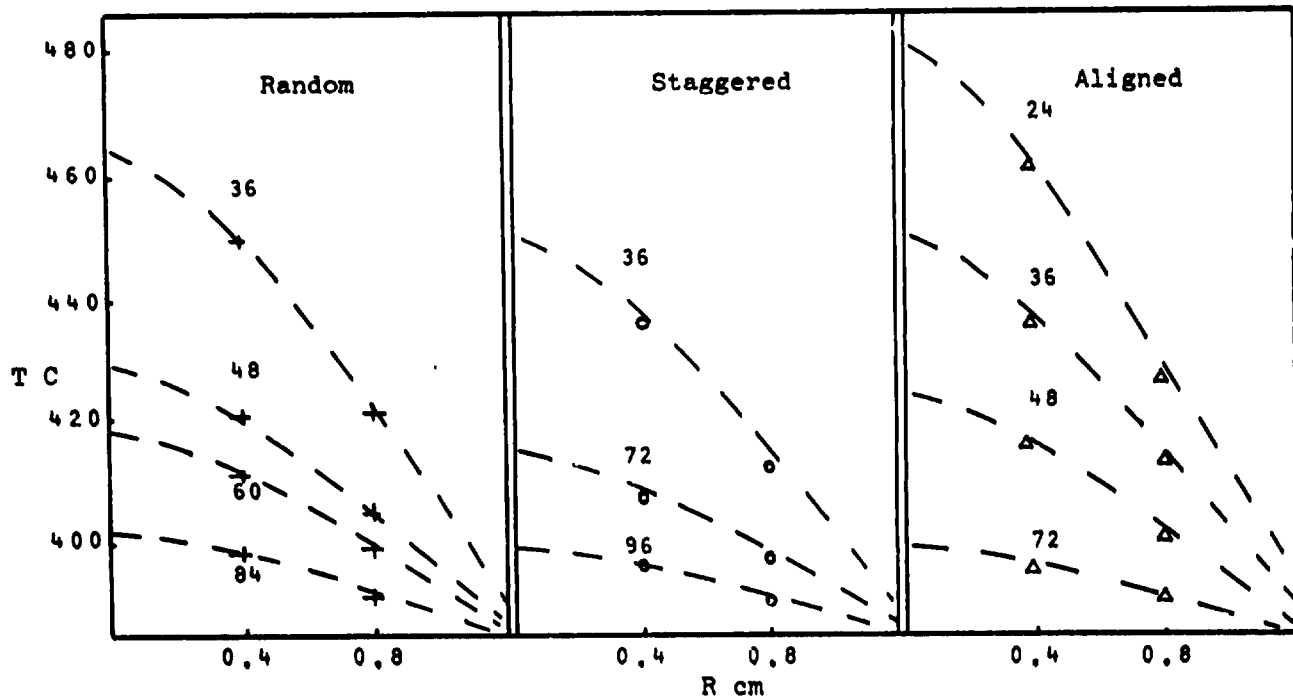


Fig. 6 Radial temperature differences for the different arrangements

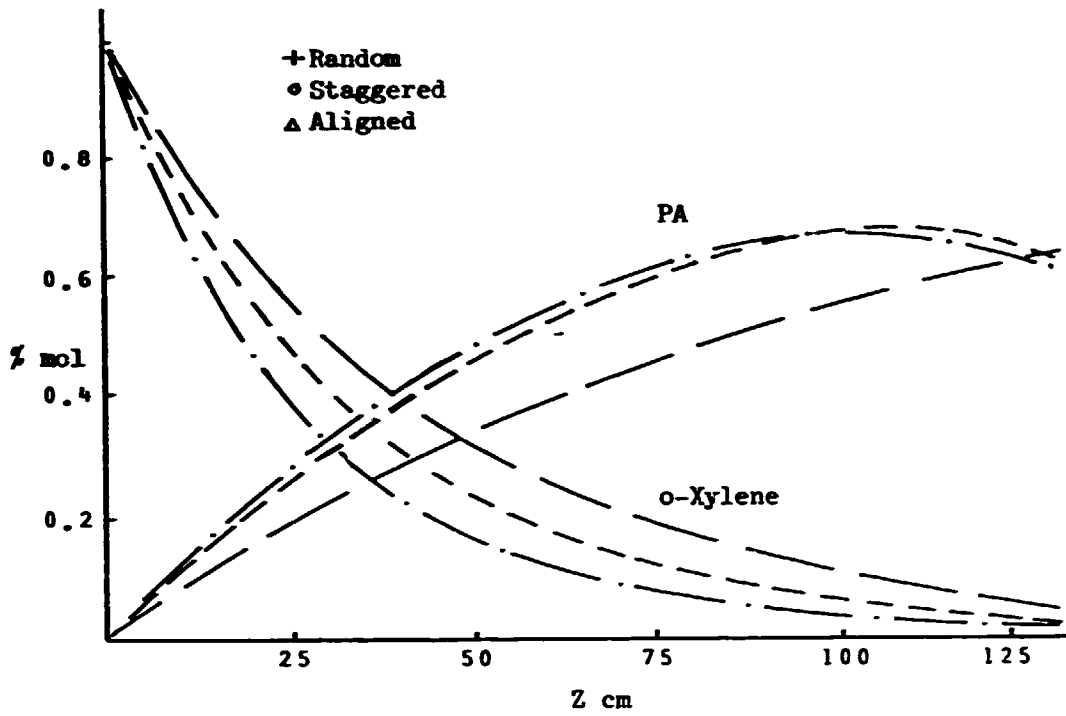


Fig. 7 Axial concentration profile for the different arrangements

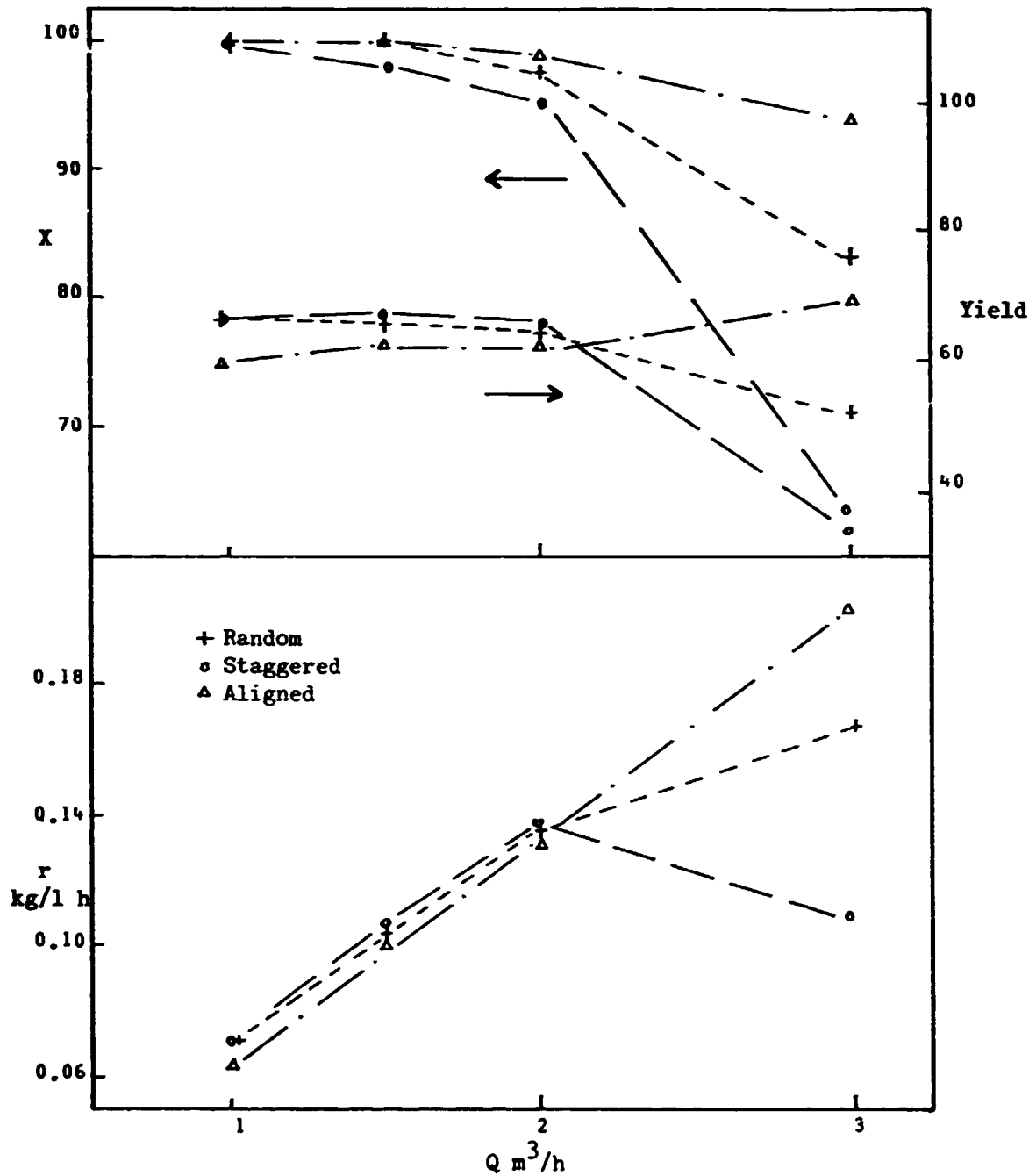


Fig. 8 Influence of the volumetric feed for the different arrangements