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DYNAMICS OF AN EXOTHERMIC REACTION
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IN A FIXED BED CATALYTIC REACTOR

by

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To My Family

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ABSTRACT

An investigation was undertaken to model the experimental results obtained for a highly exothermic reaction carried out in a non-adiabatic, non-isothermal, tubular catalytic reactor under both steady state and dynamic conditions.

The system studied was the partial oxidation of o-xylene to phthalic anhydride over commercial vanadium pentoxide catalyst. The inlet o-xylene concentration in the air stream was varied from 0.31 to 0.73 mole% (1.26×10^{-4} to 3.0×10^{-4} Kmole/m³ at 25°C) with the reactor bath temperature ranging from 340 to 355°C.

The orthogonal collocation method was extensively used to solve the two-dimensional homogeneous and heterogeneous steady state models and to facilitate estimation of the relevant parameters by implementation of a non-linear regression analysis. An anomalous effect was found over the first quarter of the reactor. Increasing the o-xylene concentration, under otherwise constant conditions, resulted in a decrease of the steady state temperature and hence the rate of heat generation. This implies that the apparent order of reaction over this region was negative. Consequently the system could not be consistently modelled using a normal first order rate of reaction expression. The simplest feasible model to demonstrate the anomalous behaviour was derived by assuming that increasing the

o-xylene concentration caused reversible deactivation of the vanadia catalyst. This resulted in a negative order of reaction at high o-xylene concentrations.

The effect of film heat and mass transfer was unimportant, up to 410°C, the maximum temperature modelled. The same degree of accuracy therefore was achieved for both the homogeneous and heterogeneous models.

Based on the steady state parameters the reaction system was solved for the dynamic case of a step change in the total gas flow rate and/or the o-xylene concentration. The continuum mathematical model of partial differential equations was solved by application of the orthogonal collocation method in all three dimensions.

The model demonstrated all the trends of the dynamic experimental results, including for an increase in the inlet o-xylene concentration, the initial small amount of right way behaviour in the axial temperature profile for the first part of the reactor; this was followed by the overall wrong way behaviour to the new steady state.

With the ever increasing demand for petroleum fuel and plastics the major source of basic raw material for the chemical industries of the world is undoubtedly crude oil and to a lesser extent natural gas. The catalytic side of the oil refining industry has developed massively since the first commercial cracking was carried out in 1936. Now heterogeneous catalysis is one of the main technologies used in the industry with reactions such as isomerisation, reforming, oxidation, hydrogenation and alkylation being possible. Such diverse products as alcohol and rubber can now be produced synthetically.

For a long time, the design of all but isothermal and the simplest adiabatic tubular reactors was impossible without scale-up from extensive pilot plant testing of the process. With the development of simple mixing cell models, the availability of heat transfer data and especially the advent of computers, the modelling of non-isothermal, non-adiabatic catalytic reactors became feasible. As computer facilities improved, solution of the relevant partial differential equations by continuum models and methods has generally superseded the mixing cell model. With improved integration algorithms progressing through the predictor-corrector, Runge-Kutta, Crank-Nicholson methods and now the orthogonal collocation method, it is possible to solve extremely complex reaction models even under dynamic conditions. The solutions however, are still very much dependent on the accuracy of the heat and mass transfer correlations as well as the

activity of the catalyst under actual operating conditions.

The aim of this study was to investigate experimentally and theoretically a tubular exothermic catalytic reactor under both steady state and dynamic conditions. This was ultimately for use as a computer controlled process in the pilot plant laboratory of the department of Chemical Engineering. Mathematical modelling was to be carried out using the orthogonal collocation method for integration radially, axially, and in the time direction, if possible, to determine the suitability of this algorithm.

The partial oxidation of o-xylene to phthalic anhydride over a vanadia catalyst was chosen, as being representative of modern catalysis technology. Other important considerations were the ease of feeding the reactants, only slow deactivation of the catalyst and a large amount of literature on the reaction at steady state conditions.

The modelling of a catalytic reactor involves the application of data on chemical kinetics, effective axial and radial diffusivity, wall heat transfer coefficients, effective thermal conductivity and heat and mass transfer coefficients. For the specific case of the oxidation of o-xylene on vanadia, the catalyst pellets are only surface coated and intraparticle effects are not important.

2.1 Kinetic Review

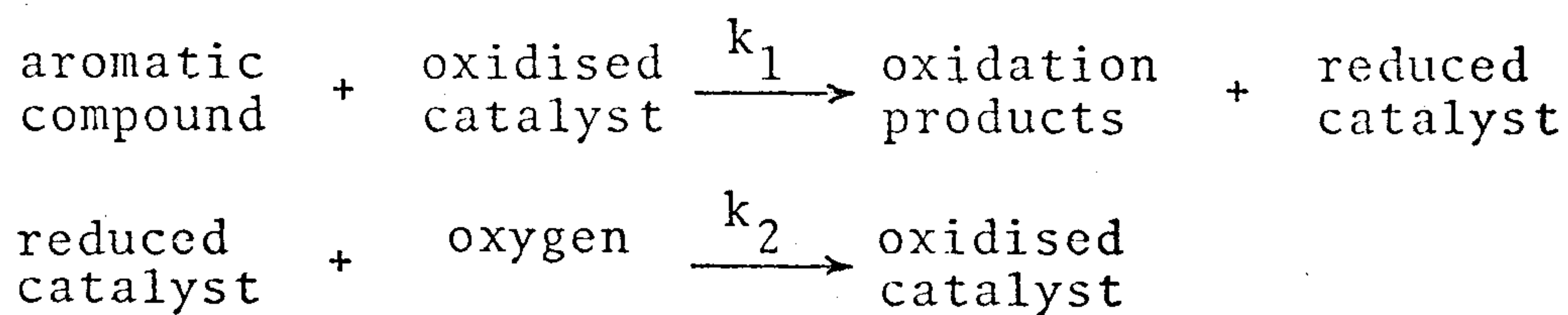
There are two main types of catalyst used for the partial oxidation of o-xylene to phthalic anhydride. The German type which has an optimum yield of approximately 75 mole% at reaction temperatures of 350-450°C, and the American type which has a slightly lower maximum yield of 70 mole%, however the rate of reaction is much faster as temperatures of 500-600°C are used. The catalysts are normally only surface coated with the support being silica in the first case and alundum or carborundum in the second. The German type catalyst is often promoted by the addition of K_2O/K_2SO_4 .

The overall rate of reaction most commonly used is the power law

$$R_r = k_r C_{O_2}^n C_r^m$$

where normally $m=1$. When the oxidation is carried out using air, the oxygen concentration, in the most extreme case for 1 mole% inlet o-xylene concentration, would only decrease from 21 to 17%. Therefore the effect of the oxygen partial pressure has usually been ignored, so that $n=0$ in the above expression.

Mars and Krevelen (3) proposed the redox model where the lattice oxygen of the catalyst is included in the reaction steps according to:



with the resulting rate of reaction

$$R_r = \frac{k_2 C_{O_2}^m k_1 C_r}{k_2 C_{O_2}^m + nk_1 C_r}$$

where n is the stoichiometric number of oxygen molecules for the reaction of one aromatic molecule. Mars and van Krevelen found a constant value for the catalyst oxidation rate constant k_2 for the oxidation of benzene, naphthalene and anthracene, with $m=1$.

Shelstad, Downie and Graydon (4) produced the steady state adsorption model (SSAM), by assuming that only oxygen is adsorbed onto the catalyst with a negligible amount of desorption. The reaction takes place between the adsorbed oxygen and the gas phase aromatic with the

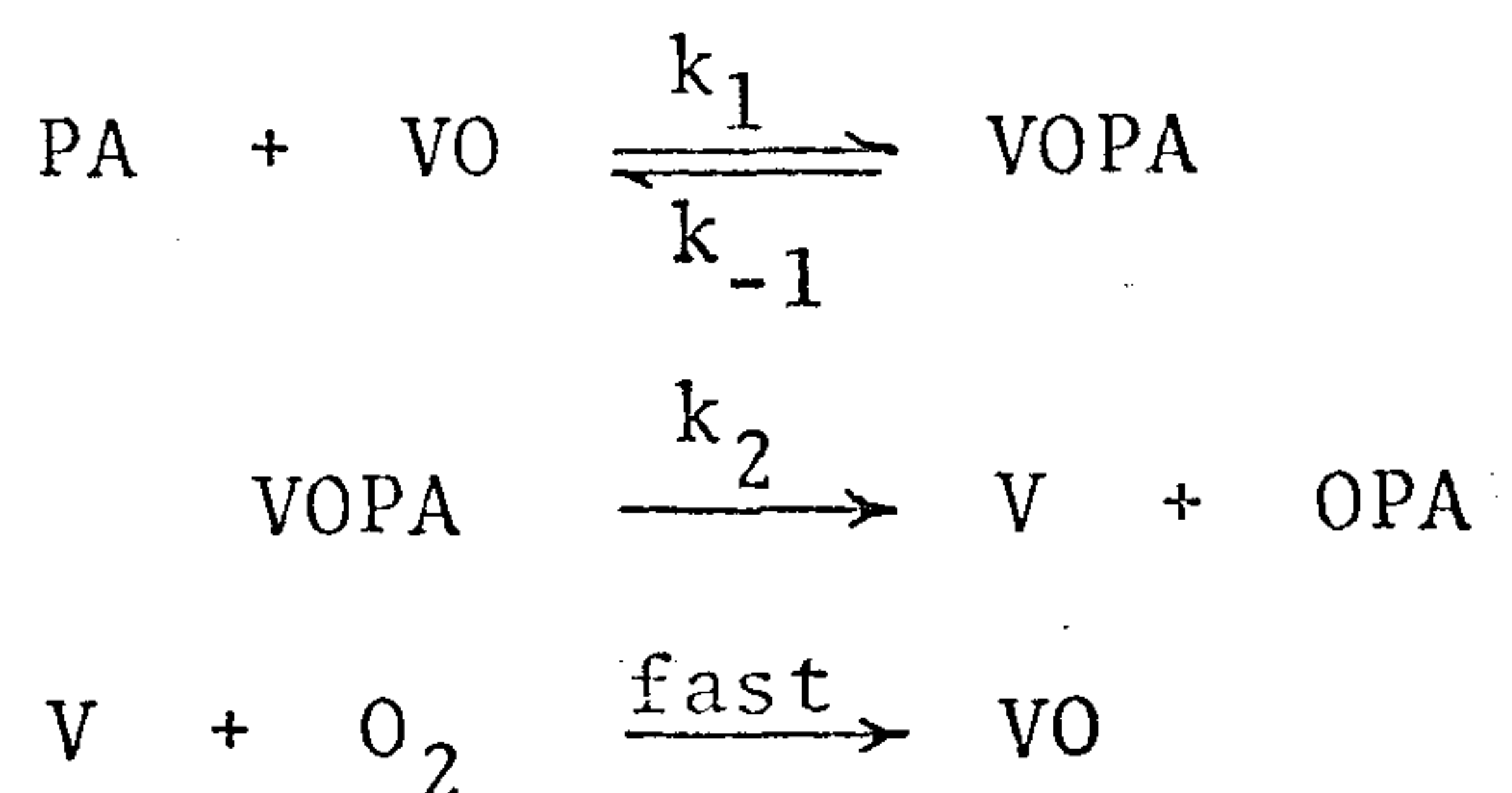
consequent rate of reaction

$$R_r = \frac{k_a C_{O_2} k_r C_r}{k_a C_{O_2} + n k_r C_r}$$

where k_a is the oxygen adsorption rate constant

k_r is the reaction rate constant.

Hughes and Adams (5) studying the vapour phase oxidation of phthalic anhydride postulated yet another model derived from the following set of equations:



with the rate of reaction

$$R_r = \frac{k_2 k_1 C_r}{k_2 + k_{-1} + k_1 C_r}$$

which simplifies to

$$R_r = \frac{A C_r}{1 + B C_r}$$

Originally, the model was developed using lattice oxygen but it could equally apply to adsorbed oxygen.

As the forms of the rate expression for the redox model with $m=1$ and the SSAM are identical, discrimination between the models cannot be done by simple kinetic studies. The Hughes and Adams form can be distinguished by varying the oxygen partial pressure, but when this is

constant, all three heterogeneous rate expressions are identical. In the extreme case, these models can give an order of reaction for the aromatic varying from 0 to 1 as the concentration of the aromatic decreases to zero.

Cameron, Farkas and Litz (6) found exchange of isotopic oxygen between the gas phase and the vanadia catalyst over all the temperature range that they investigated, 445 to 554°C. The exchange rate was independent of the oxygen partial pressure and had an activation energy of 1.88×10^8 KJ/mole. They proposed either the dissociation of oxygen molecules or the loosening of V-O bonds was involved. Margolis (7) supported this, adding that the exchange rate only becomes observable above 435°C.

Clark and Berets (8) studying the electronic behaviour of vanadium pentoxide, state that the presence of an electron donating agent such as ethylene or o-xylene prevents the formation of the oxygen barrier which would normally form in an atmosphere of oxygen alone. The exchange of oxygen at the surface during a catalytic reaction should then be much faster than has previously been indicated by measurement of oxygen absorption alone.

Simard and co-workers (9) demonstrated that there is sufficient lattice oxygen present in the catalyst to

react with o-xylene at 460°C, over freshly prepared vanadia, in a stream of nitrogen, resulting in a decrease in the oxidation state of the catalyst. This shows that chemically bound oxygen can take place in the reaction. For oxygen adsorption by slightly reduced catalyst, Simard found a square root dependence on the oxygen partial pressure. Roiter (10) however, found no evidence of exchange of isotopic oxygen for the oxidation of naphthalene in the temperature range 340-390°C. Boreskov (11) states that adding promoters to the catalyst can greatly increase the catalytic activity in relation to the exchange of molecular oxygen, for example, adding 10 mole% cesium sulphate, which is a stronger promoter than potassium sulphate, results in a hundredfold increase in the rate of exchange.

Out of all this conflicting evidence, as well as the large variations possible in the formulation of a promoted catalyst, it is best to assume both adsorbed and chemically bound oxygen are active species in the partial oxidation of o-xylene to phthalic anhydride. The general forms of the models so far produced cannot make this distinction, therefore this assumption is in order.

Shelstad (4) and Juusola and co-workers (12), studied the reaction of naphthalene to phthalic anhydride, and o-xylene to o-tolualdehyde respectively. Both workers tried Langmuir-Hinshelwood models where both the aromatic and oxygen molecules are reversibly adsorbed onto the catalyst.

$$R_r = \frac{k_r k_1 k_2 C_{O_2} C_r}{(1 + k_1 C_{O_2} + k_2 C_r)^2}$$

For Shelstad's work, the Langmuir-Hinshelwood model gave a slightly better fit, however the extra complexity of the model was not considered to be practicable and both groups of workers settled for the SSAM. Juusola also rejected various other models including the SSAM with a square root dependence of oxygen partial pressure caused by the supposed dissociative adsorption of oxygen by the catalyst.

Juusola modified the SSAM to

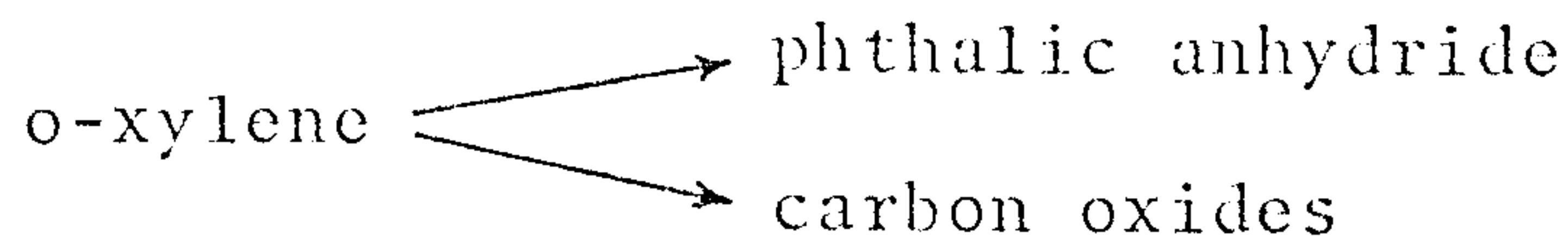
$$R_r = \frac{k_a C_{O_2} k_1 C_r}{k_a C_{O_2} + \sum_{i=1}^N n_i k_i C_{r_i}}$$

where the summation term is for all the reacting aromatic species, especially those involved in series reactions. This idea can conceivably be extended to the bimolecular Langmuir-Hinshelwood reaction.

$$R_r = \frac{k_r k_1 k_2 C_{O_2} C_r}{(1 + k_1 C_{O_2} + \sum_{i=1}^N k_{i+1} C_{r_i})^2}$$

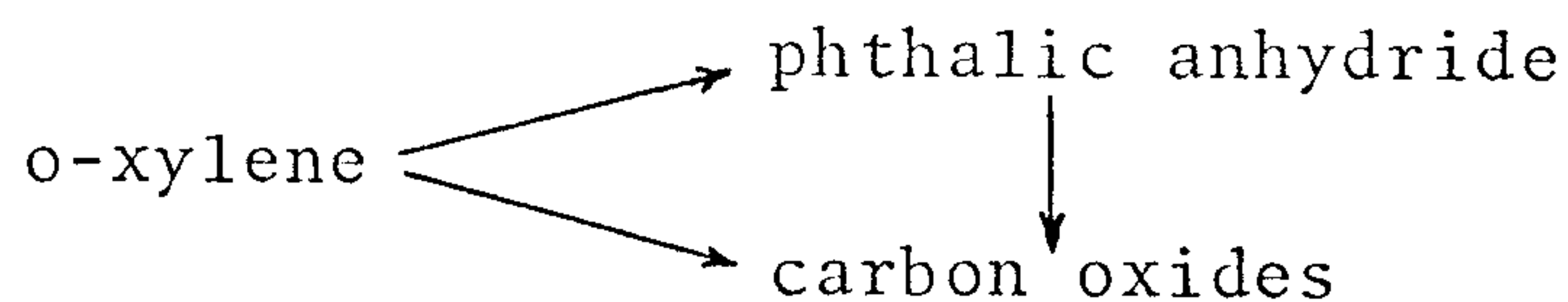
A multitude of reaction schemes exist in the literature for the reaction of o-xylene over vanadia type catalysts. These are well described by Ellis (13). Only the simplest schemes will be presented here.

The basic model, used by many workers, assumes two parallel reactions, first order with respect to o-xylene and both having the same activation energy.

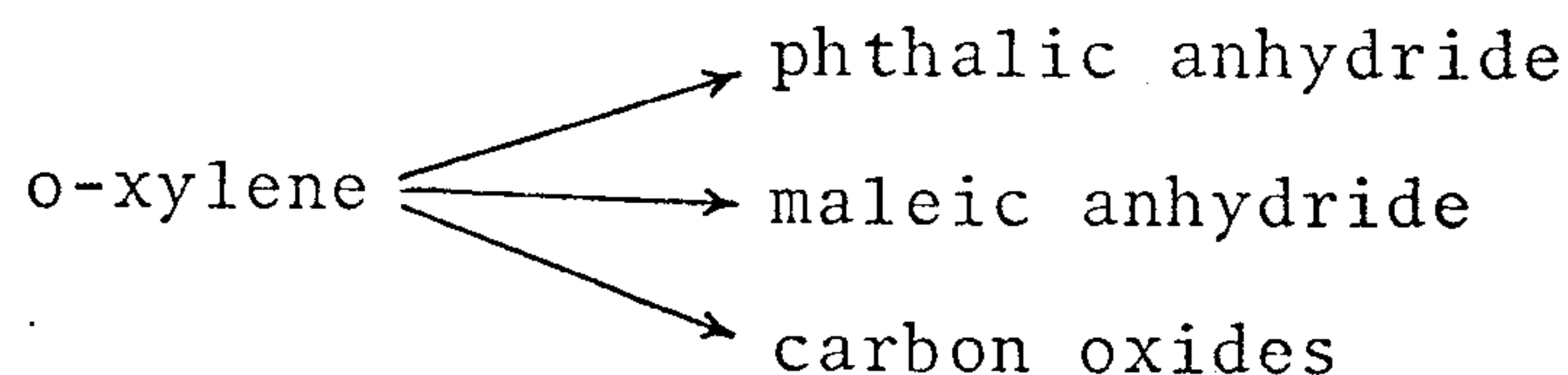


This explains the constant selectivity of the system over a wide range of temperatures found by most workers.

A slightly more complex model, a triangular scheme of first order reactions, was developed by Froment (14) as being fairly representative of the gas phase oxidation of o-xylene over vanadium pentoxide.



Aliev (15) and Pant and Chanda (16) both postulated identical schemes involving only parallel reactions.

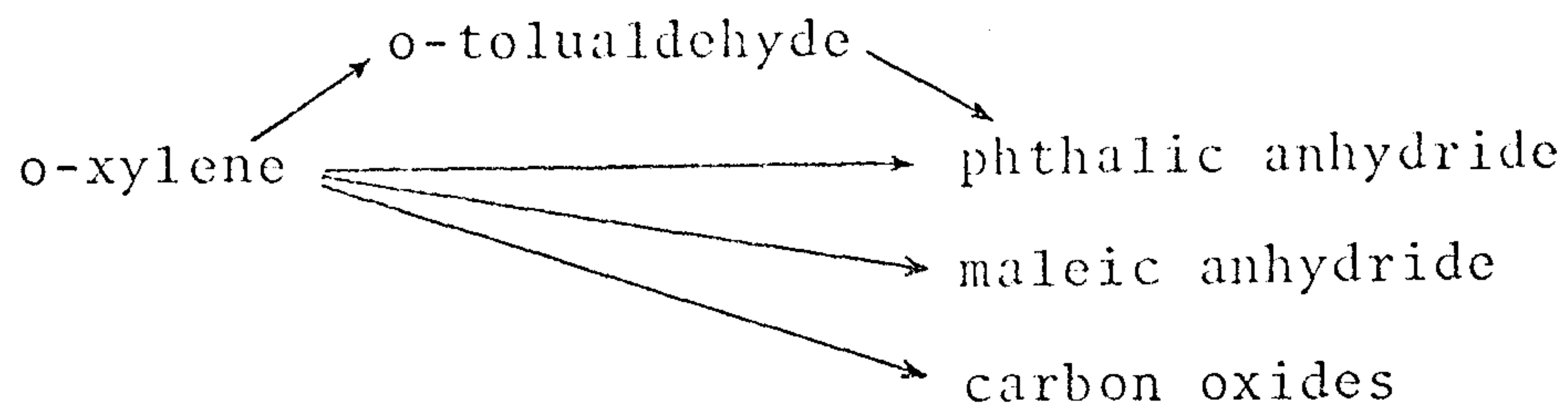


Pant and Chanda developed the rate of reaction expression in the form of a summation of the SSAM derived by Juusola.

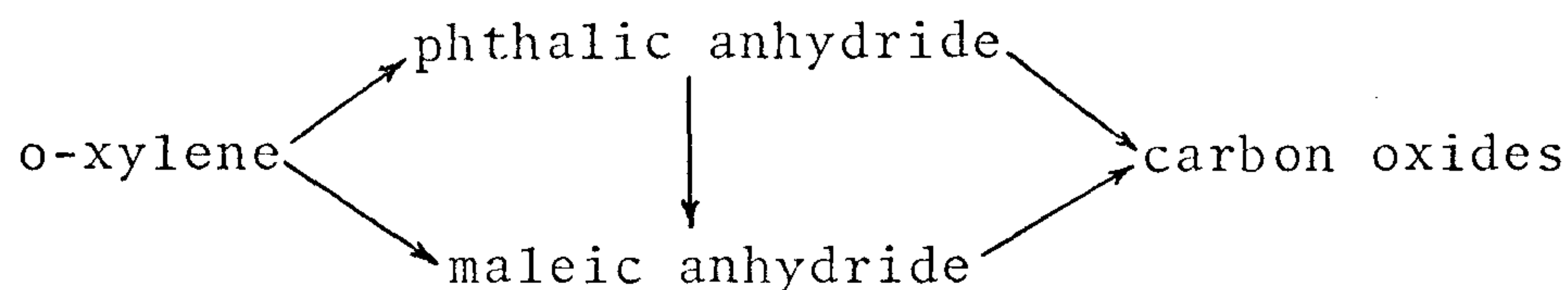
$$R_r = \frac{(k_1 + k_2 + k_3) K_4 C_{O_2} C_r}{K_4 C_{O_2} + 3 k_1 C_r + 7.5 k_2 C_r + 10.5 k_3 C_r}$$

Where the numbers 3, 7.5 and 10.5 are the stoichiometric amounts of oxygen necessary for the respective reaction. The reaction expression however, reduces to the normal SSAM form, as the activation energy of the three reactions are the same and there are no series reactions present in the scheme.

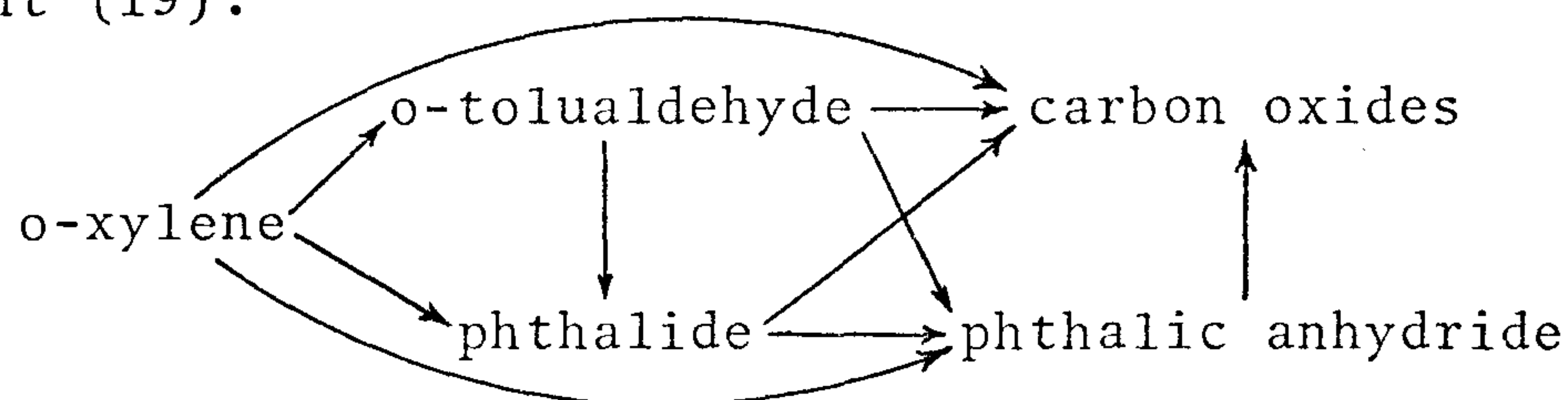
Dixon, Longfield and Emmet (17) reporting the unpublished work of Simard give the following network.



Carra and Beltram (18) found no traces of o-tolualdehyde and concluded that their data could be represented by the following scheme with no direct o-xylene combustion.



The following network was proposed by Herten and Froment (19).

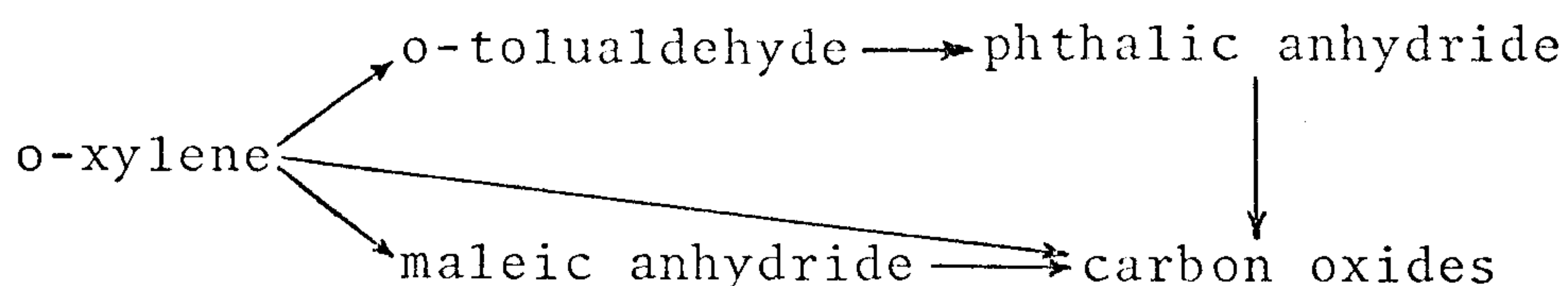


The overall rate of o-xylene disappearance was modelled equally well by either the power law or the Mars and van Krevelen form with the exponent m equal to 0.6.

A scheme similar to that of Herten and Froment was devised by Vanhove and Blanchard (20), with no direct reaction of o-xylene to either phthalide or to phthalic anhydride.

Boag and co-workers (21) also proposed a network similar to that of Herten and Froment, but with no further oxidation of phthalide. They add that as mutual inhibition effects are known to be important for this system, as demonstrated by Lubarskii and co-workers (22), it is possible that the product distribution may not be a unique

function of conversion. The results of workers therefore who have oxidised various intermediates are not necessarily correct especially as regards the rate of reaction. The results of Boag were derived by a statistical approach from the reaction of o-xylene alone, although only a maximum phthalic anhydride selectivity of 45% was achieved. Novella and Bennloch (23,24,25) deduced the model



Further complex schemes for the oxidation of o-xylene or the reaction of various intermediates have been developed by Lyubarskii and co-workers (22), Bernadini and Ramacchi (26) and Vrbaski and Matthews (27,28) with even more intermediates namely o-methyl benzaldehyde, o-toluic acid, per-o-toluic acid and benzoic acid.

Many of the reaction schemes show the further oxidation of phthalic anhydride. Hughes and Adams (5) and Ioffe and Sherman (29) agreed that phthalic anhydride underwent direct combustion to carbon oxides and partial oxidation to maleic anhydride. Watt (30) showed that this was important in his kinetic studies on the reaction of o-xylene using a spinning basket reactor, due to the long residence times used. Normally however, even in long packed bed reactors this effect is not important as contact times are of the order of 1 second.

Ignoring the results where there have been obvious

mass transfer limitations on the rate of reaction the activation energy for the o-xylene reaction is in the range 0.92×10^8 to 1.17×10^8 KJ/Kmole, with most oxygen adsorption or kinetic activation energies between 1.05×10^8 and 1.25×10^8 KJ/Kmole.

Some workers comment on a reduction in the rate of reaction at high aromatic concentrations. In most cases the full catalytic activity was restored by decreasing the aromatic concentration or by passage of an air stream over the catalyst. Simard (9) found that the vanadia catalyst reversibly deactivated at an o-xylene concentration of 3.3 mole%, however he did not investigate the range between 1.1 and 3.3%. Ross and Calderbank (31) similarly had a loss of catalytic activity at naphthalene concentrations greater than 1.0 mole% at 353°C as did Calderbank and co-workers (32) at o-xylene concentrations greater 1.6%. Calderbank (33) using a spinning basket catalytic reactor, found that the order of the rate of reaction, initially nearly one with respect to o-xylene, decreased to zero in the concentration range 0.6 to 1.1% at 400°C and then became negative at higher concentrations. A good fit for the data at 400°C can be obtained by a simplified form of the Langmuir-Hinshelwood expression, where the oxygen partial pressure is nearly constant and can therefore be included in the rate constants

$$R_r = \frac{k_r C_r}{(1 + k_1 C_r)^2}$$

$$\text{where } k_1 = 1.35 \times 10^2$$

$$k_r = 1.71 \text{ Kmole}/(\text{Kg cat}).s$$

Shelstad (4) and Juusola (12) at high concentrations of the aromatics they studied, showed that the order of the reaction decreased to zero, or may even have become negative, in the second study, when naphthalene and o-xylene concentrations were above 1.0% and 1.2% respectively. As mentioned previously however, they rejected the bimolecular Langmuir-Hinshelwood model which would explain this effect in favour of the simpler SSAM.

Lyubarskii and co-workers (22) studying the oxidation of o-xylene to phthalic anhydride and the reaction of various intermediates, found that the oxidation of maleic anhydride proceeded as a simple first order reaction. When phthalic anhydride was present however, the reaction was inhibited by the adsorption of phthalic anhydride on the catalyst.

$$R_r = \frac{k_r C_{ma}}{1 + b C_{pa}}$$

where b is an adsorption rate constant. For a complete description of the oxidation of o-tolualdehyde, an expression similar to the modified form of the SSAM, proposed by Juusola, was necessary where

$$R_r = \frac{k_r C_{tol}}{1 + b_1 C_{tol} + b_2 C_{ma} + b_3 C_{pa}}$$

The adsorption of phthalic and maleic anhydrides however, was much weaker than that of the o-tolualdehyde so that these two terms in the denominator could be ignored resulting in the rate of reaction equation originally derived by Hughes and Adams (5).

Roiter and co-workers (34) claimed that the naphthoquinone concentration, a by-product in the reaction of naphthalene to phthalic anhydride, had a retarding effect on its own rate of formation from the naphthalene and proposed the empirical rate of reaction expression;

$$R_r = \frac{k_1 C_n C_{O_2}}{C_{nq}^{0.6} (1 + k_2 C_n)}$$

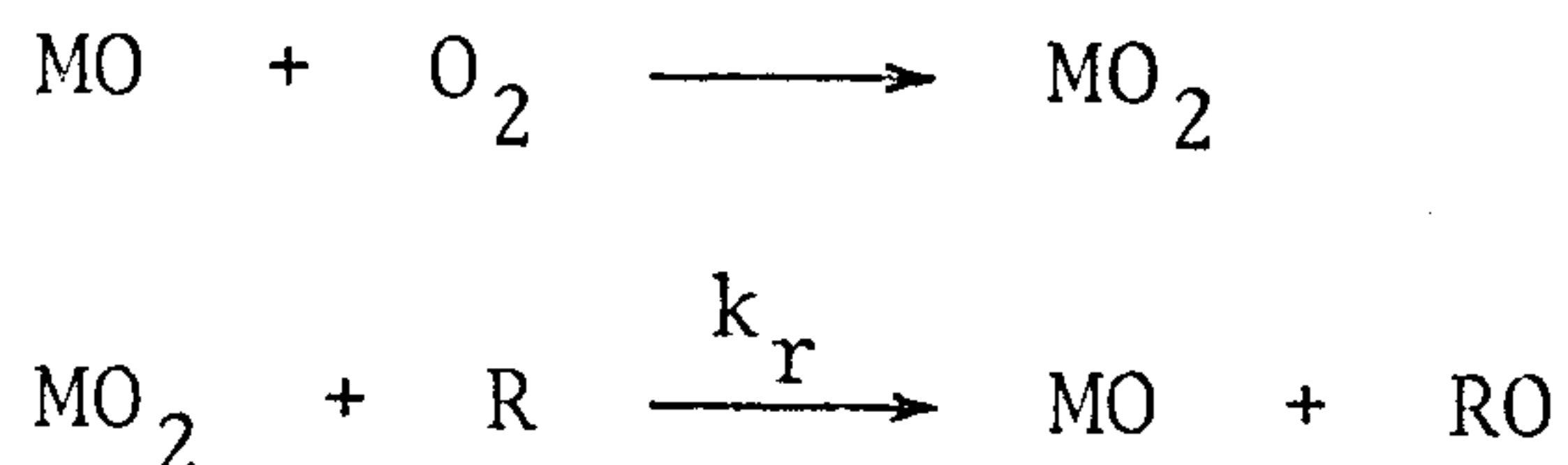
They unsuccessfully tried modelling the system with a series reaction type and a unimolecular Langmuir-Hinshelwood type, however they do not report trying a bimolecular Langmuir-Hinshelwood model.

The decrease in the order and the rate of reaction at high aromatic concentrations is caused either by a preferential adsorption on the catalyst of the hydrocarbons present, resulting in the exclusion of the oxygen, which can be explained by the Langmuir-Hinshelwood model, or by a reduction in the oxidation state of some or all of the catalyst present resulting in a decrease in activity.

Conversely Hughes and Adams studying the reaction of phthalic anhydride found an increase in the rate of reaction when the oxygen concentration was less than 10%; however above this value the rate of reaction was found to be independent of the oxygen concentration. This was explained by the vanadia catalyst being reduced to a lower oxidation state which was more active for the oxidation of phthalic anhydride.

Little work has been published on the active oxidation state of the vanadia catalyst. Simard (9) states that for o-xylene reaction V_2O_5 and $V_2O_{4.34}$ are active, while Volf'son (35) working on naphthalene oxidation claims that only V_2O_4 is active. Schaefer (36) using benzene agrees that V_2O_4 is active and adds that $V_2O_{4.34}$ is slightly active. Farkas (37) claims that this variation in active catalyst species is due to the different nature of the reactions taking place. There is no ring breaking in the o-xylene reaction and for the naphthalene and benzene reactions, the rings break in a dissimilar way.

Ioffe (38) states that the phase composition of the operating catalyst is completely determined by kinetic rather than thermodynamic parameters and postulates the reactions



Reaction of the aromatic can also occur with adsorbed oxygen on the reduced MO phase giving the overall rate of reaction expression as the sum of two terms.

$$R_r = k (1 - \xi) \theta_{O_2} f(C_r) + k_r \xi f'(C_r)$$

where ξ is the fraction of MO_2 present

θ_{O_2} is the fractional surface covering of adsorbed oxygen

A steady state occurs when the two phases are in kinetic equilibrium according to:

$$k_1 \phi(\xi) f_1(C_r) = k_2 \phi(1-\xi) f_2(C_{O_2})$$

Ioffe and Lyubarskii (37) studied the partial oxidation of benzene to maleic anhydride over a vanadium pentoxide catalyst in a recycling differential reactor. It was found that the presence of maleic anhydride retarded the reaction and that at oxygen partial pressures less than 0.1atm the reaction was second order in oxygen while at higher concentrations the reaction was zero order.

For the theoretical analysis the following assumptions were made:

- 1 The major portion of benzene oxidation was by the oxygen adsorbed on the surface of the V_2O_5 .
- 2 A minor portion of benzene oxidation was by the oxygen of the V_2O_5 lattice.
- 3 Maleic anhydride is more strongly adsorbed onto the surface of the V_2O_5 than oxygen.
- 4 The benzene oxidation rate by adsorbed oxygen is much greater than that by the lattice oxygen.

These assumptions enabled the second term of Ioffe's original rate of reaction expression to be neglected. By extending the theory to include the diffusion of oxygen vacancies through the catalyst the following simplified equation results.

$$R_r = k f(C_{O_2}) \frac{C_{bz}}{1 + k_a C_{ma}}$$

where

$$f(C_{O_2}) = k_1 C_{O_2}^2 \quad \text{at low oxygen concentrations}$$

$$f(C_{O_2}) = k_2 \quad \text{at high oxygen concentrations}$$

which was approximated by:

$$R_r = k' f(C_{O_2}) \frac{C_b^\alpha}{C_{ma}^\beta} \quad \alpha \text{ and } \beta < 1$$

This model demonstrates all effects that were reported, including the retardation of the reaction by the presence of maleic anhydride, however at no point was a negative order of reaction found.

2.2 Mathematical Modelling

Many models have been formulated to describe the characteristics, and facilitate the design, of fixed bed catalytic reactors. The partial oxidation of o-xylene to phthalic anhydride in a non-isothermal, non-adiabatic tubular catalytic reactor at a reaction rate comparable to industrial reactors, produces a large radial temperature variation. This is due to the high exothermic heat of reaction and the need for continuous heat transfer through the wall to avoid excessive bed temperatures which may decrease or destroy the activity of the catalyst.

Froment (2,40) has shown, for the o-xylene reaction, that there is a considerable difference in the theoretical temperature profiles between calculations carried out using one and two dimensional single phase models. Consequently one dimensional models have not been used in this study, as the reactor used for the experiments was of semi-industrial size.

Carberry and Wendel (41) concluded that axial dispersion of heat and mass was important only for shallow beds and is negligible for bed lengths greater than 50 pellet diameters. Axial dispersion of both heat and mass effects have initially been ignored in this study as the bed length was 120 pellet diameters.

In the studies of reverse operation of catalytic reactors carried out by Berty and co-workers (42) and Venkatachalam and co-workers (43) it is obvious that axial dispersion of heat is important to propagate the reaction zone towards the inlet of the bed. The temperature however, in these cases was normally much greater than 400°C, therefore radiation effects would be far more important than for the o-xylene reaction, as well as the conductivity of the packed beds being much greater than that of the silica catalyst used in these experiments.

In order to understand the literature on the mathematical modelling, the partial differential equations governing the system studied will be presented here. For a detailed derivation of the various dimensionless equations presented and the symbols used, see appendices I and V respectively.

Two types of steady-state two dimensional models have been used, the simplest being the homogeneous or single phase case where temperatures and concentrations at the pellet surface are assumed to be equal to the bulk gas temperature and concentration. This leads to the following dimensionless partial differential equations for energy and mass balances.

$$\frac{\partial T}{\partial z} = \beta g(T, C) + \alpha \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right)$$

$$\frac{\partial C}{\partial z} = - \frac{g(T, C)}{C_0} + \gamma \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right)$$

with boundary conditions

$$\frac{\partial T}{\partial r} = - Bi(T - T_c) \quad \text{at } r = 1$$

$$\frac{\partial C}{\partial r} = 0 \quad \text{at } r = 1$$

$$T = C = 1 \quad \text{at } z = 1$$

As the catalyst pellets used were only surface coated with the active agents, intraparticle effects are eliminated.

The other two dimensional model considered was the heterogeneous or two phase case where the temperatures and concentrations at the surface of the pellet are not equal to the bulk gas temperatures and concentrations, but are governed by these dimensionless equations:

Energy Balance

$$\beta g(T_p, C_p) = St_{ht}(T_p - T_b)$$

$$\frac{\partial T_b}{\partial z} = St_{ht}(T_p - T_b) + \alpha \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_b}{\partial r} \right)$$

Mass Balance

$$- \frac{g(T_p, C_p)}{C_0} = St_{mt}(C_p - C_b)$$

$$\frac{\partial C_b}{\partial z} = St_{mt}(C_p - C_b) + \gamma \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_b}{\partial r} \right)$$

with boundary conditions

$$\frac{\partial T_b}{\partial r} = - Bi(T_b - T_c) \quad \text{at } r = 1$$

$$\frac{\partial C_b}{\partial r} = 0 \quad \text{at } r = 1$$

$$T_b = C_b = 1 \quad \text{at } z = 1$$

where the subscripts p and b refer to pellet and bulk conditions respectively. No solid phase heat transfer has been directly considered i.e. no intrapellet, pellet to pellet, or pellet to wall, only solid to gas, gas phase and gas to wall heat transfer. The solid effects however, are indirectly included in the overall effective thermal conductivity and what is really an effective wall heat transfer coefficient. This is a contradiction as the model is therefore not a complete heterogeneous model. Considering solid heat transfer separately would mean the introduction of an extra effective conductivity and wall heat transfer coefficient. Most literature correlations however, consider all the heat transfer effects to be lumped into a single overall effective conductivity and a wall heat transfer coefficient. Even for these parameters there is much variation (see chapters 2.4 and 2.5) so that the addition of two extra parameters cannot be justified.

The packed bed was assumed to operate at atmospheric pressure with negligible pressure drop through the bed. Plug flow has been assumed throughout all the models in this study. No radial variation in velocity has been considered as this appreciably complicates the equations. There is however, partial compensation for this effect, as it is inherent in the experimentally obtained values of the effective thermal conductivity and wall heat transfer coefficient. Neither of these parameters have been correlated by any workers for radial variation of the flow rate.

As axial dispersion has been neglected for the modelling, there are no axial second derivatives. This reduces the partial differential equations for both models considered from elliptic to the more readily solveable parabolic form.

These partial differential equations have commonly been solved by finite difference methods, especially that of Crank-Nicolson, where first and second partial derivatives are approximated by a form of the solution at two and three points respectively, i.e. linear and parabolic approximations respectively. Therefore at best, the solution radially and axially, is a series of interconnected parabolas and straight lines respectively. Alternatively the orthogonal collocation method can be used where the whole set of radial points are fitted by a symmetrical $2N$ th order polynomial. The number of internal collocation points is N , the positions of these being selected according to the procedures originally defined by Villadsen and Stewart (44). This is analagous to Gaussian quadrature, which is exact for a polynomial of order $2N$. For a full derivation of the orthogonal collocation method and its application, see appendices II and III respectively. The first and second partial derivatives are then obtained by multiplying a weighting vector by the solution vector so that both derivatives are approximated by the respective derivative of the polynomial solution. This gives rise to more accurate solutions than the Crank-Nicolson method, meaning fewer solution points are necessary for comparable accuracy,

therefore decreasing computer storage requirements.

When the collocation method is applied radially, the radial derivatives are replaced by constant terms and the partial differential equations are reduced to the ordinary differential form. Normally these equations have been integrated by finite difference methods e.g. Runge-Kutta (45) or Euler (46), but it is possible to apply the orthogonal collocation method again axially in steps (47). The solutions axially are approximated by (N+1)th order polynomials and for the dynamic case, this method can be applied yet again in the time direction.

For the dynamic model, the dimensionless partial differential equations are:

Energy Balance

$$\beta g(T_p, C_p) = St_{ht}(T_p - T_b) + \xi \frac{\partial T_p}{\partial t}$$

$$\frac{\partial T_b}{\partial z} = St_{ht}(T_p - T_b) + \alpha \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_b}{\partial r} \right)$$

Mass Balance

$$- \frac{g(T_p, C_p)}{C_o} = St_{mt}(C_p - C_b)$$

$$\frac{\partial C_b}{\partial z} = St_{mt}(C_p - C_b) + \gamma \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_b}{\partial r} \right) - \epsilon \frac{\partial C_b}{\partial t}$$

Where the boundary conditions are the same as for the heterogeneous case and the temperature and concentration profiles are defined at time $t = 0$.

A packed bed reactor has two characteristics response times, one for concentration changes of the order of a few seconds, or residence times, and the other for the

bed temperature changes of the order of a few minutes.

Due to the difference in magnitude of the two responses, the two transients can be separated into two models to simplify the calculations. The first for concentration changes with pseudo-constant temperature and the second for the temperature transients with the concentration going through a series of pseudo-steady states following the temperature profile. The equations governing the concentration transient, after a radial orthogonal collocation substitution, are most easily solved by the method of characteristics. Temperature variations along the bed can be included by bending the characteristic lines as the solution progresses. The orthogonal collocation method could be used axially and in the time direction although the computational time may be excessive. It cannot however accurately handle a discontinuity in a variable e.g. when the concentration undergoes a step change.

For the temperature transient, the original three dimensional concentration partial differential equation is replaced by the steady state heterogeneous concentration equation, resulting in all parabolic equations which can be solved by finite difference methods, or a mixed or complete orthogonal collocation method. As large time steps (much greater than the residence time) can be taken, any concentration discontinuity can be overstepped and does not affect the orthogonal collocation method.

2.3 Reactor Dynamics

Very little work has been reported for combined experimental and theoretical investigations of realistic pilot plant exothermic tubular reactors under dynamic conditions. Most workers have dealt with reactors that are nearly adiabatic or have studied the simple reaction of hydrogen and oxygen over a supported platinum catalyst.

Simulations of packed bed reactors under dynamic conditions, using a series of continuous stirred tank reactors, have been developed by M^CGuire and Lapidus (48), Vanderveen, Luss and Amundsen (49) and Elnashaie and Cresswell (50) where the size of each mixing cell is approximately that of a catalyst pellet, or the void between pellets. To obtain a converged steady state solution it may be necessary to decrease the cell size until it becomes meaningless so that a continuum model based on the solution of the ordinary or partial differential equations describing the reactor, is more appropriate. In the model of M^CGuire and Lapidus, where multiple steady states were possible, as each row of mixing cells moved from the lower to the higher steady state, a discrete heat wave passed along the reactor. This effect has never been found experimentally and shows a spurious result in using the mixing cell model.

Berty and co-workers (42) used both the discrete mixing cell and continuum models, the latter being solved by a predictor-corrector method to model their experiments on the backward migration of the reaction zone in an

adiabatic reactor. Although the fit obtained for the experimental data was poor, the trends were demonstrated.

Lui and Amundson (51,52,53), using continuum one-dimensional models, integrated by the method of characteristics, investigated the stability of adiabatic and non-adiabatic packed bed reactors. Heat and mass transfer resistances were lumped at the pellet surface, with an effectiveness factor being applied to account for intraparticle reaction. From these models multiple steady state situations were demonstrated.

Hansen and Jorgensen (54) obtained good agreement between their theoretical and experimental results for the hydrogen/oxygen reaction on non-porous pellets in an adiabatic reactor although they used a homogeneous one-dimensional model with all the heat transfer effects lumped into a total Peclet number. The model was solved by applying the orthogonal collocation method axially to reduce the partial differential equations to ordinary differential equations which were then integrated by a 4th order Runge Kutta method in the time direction. This paper was a continuation of the earlier theoretical simulations of Hansen (55,56). In these papers however, heterogeneous one-dimensional adiabatic models were used to describe the behaviour of packed beds of porous catalyst pellets under dynamic conditions. Hansen divided the solution of the dynamic case into two parts. The fast response dynamic concentration profiles were solved at constant bed temperature by the application of the orthogonal collocation

method for the internal pellet profiles, followed by the method of characteristics axially and a predictor-corrector method in the time direction. The slow response dynamic temperature profiles were solved by assuming that the concentration profiles went through a series of pseudo-steady states, so that only the heat balance equations had to be solved in the time direction, and the concentration profile at any time step was only dependant on the temperature profile and the inlet concentration at that time. This was solved as previously by the orthogonal collocation method and then by the Runge Kutta method axially and a predictor-corrector method in the time direction. The response time of the fast concentration profiles was found to be 2-3 seconds and the slow temperature profile 1000-1500 seconds.

Hoiberg, Lyche and Foss (57) studied the dynamics of the hydrogen/oxygen reaction under non-isothermal and non-adiabatic conditions demonstrating the classical initial wrong way behaviour for a 20°C decrease in the inlet temperature of 100°C. The frequency response of the reactor was rigorously studied over a wide range of frequencies. In all cases, the Crank-Nicolson method was used to solve the differential equations.

Elnashie and Cresswell (50) and Karanth and Hughes (58) modelled first order reactions for porous catalyst pellets under dynamic conditions, demonstrating that for porous pellets the response speed is proportional to the Lewis number as is the overshoot. The Lewis number is defined as:

$$Le = \frac{\rho_s C_p D_p}{k_p}$$

where C_p = specific heat capacity of catalyst

D_p = diffusivity of reactant inside pellet

k_p = pellet conductivity.

Karanth and Hughes investigated the dynamics of the hydrogenation of toluene over a supported nickel catalyst in a nearly adiabatic reactor. Consequently they used a one-dimensional model and utilised the limiting non-key component effect to simplify the solution of the two phase equations. Their model is in poor agreement with their experimental results, but they do demonstrate the trend. The transients that were considered were from no reaction to final steady state which took approximately 50 minutes. Unfortunately however, the inlet temperature varied over this interval.

Stewart and Sorenson (59) modelled the oxidation of o-xylene to phthalic anhydride on porous catalyst pellets, based on Froment's (14) triangular scheme of first order reactions under dynamic conditions, using a two-dimensional heterogeneous model. This was solved by applying the orthogonal collocation method to both the intraparticle and radial profiles and finite difference expressions axially and in the time direction. The collocation points for this model were calculated depending on the value of various dimensionless groups at the boundary conditions by formulas given. It is claimed that this allows good accuracy to be achieved with fewer collocation points. The Newton Raphson form was used to quasi-linearise the kinetic expressions. No experimental work was carried out.

2.4 Effective Radial Conductivity Correlations

The correlations in the literature vary greatly depending mainly on the nature of the solid packing, whether metallic or non-metallic, spherical or cylindrical. The oxidation of o-xylene is unusual in that the reactor diameter is normally 25mm with a pellet to tube diameter ratio of around 0.25 to facilitate good heat transfer to limit the hot spot temperature. Most of the experimental work on heat and mass transfer parameters has been carried out for tube diameter ratios less than 0.25. In this study a reactor of diameter 15.59mm with a diameter ratio of 0.268 was used.

Effective radial conductivity correlations normally take the form

$$\frac{k_e}{k_g} = \frac{k_e^0}{k_g} + \phi \text{ Re } \text{Pr}$$

where the first term k_e^0/k_g is the contribution of the stagnant effective conductivity representing the effects of both fluid and solid conductivities, particle size, radiant heat transfer and void fraction. The second term is the fluid flow contribution with the Reynolds number based on the pellet diameter.

Kunii and Smith (60) derived the following theoretical equation for predicting the stagnant conductivities in packed beds of unconsolidated particles:

$$\frac{k_e^0}{k_g} = \epsilon \left(1 + \beta \frac{h_{rv} D_p}{k_g} \right) + \frac{\beta(1 - \epsilon)}{\frac{1}{\phi} + \frac{h_{rs} D_p}{k_g} + \gamma \frac{k_g}{k_s}}$$

where radiation between voids is given by

$$h_{rv} = 0.1952 \frac{\rho}{2-\rho} \left(\frac{T+273}{100} \right)^3$$

radiation between surfaces by

$$h_{rs} = \left(\frac{0.1952}{1 + \frac{\epsilon}{2(1-\epsilon)} \frac{1-\rho}{\rho}} \right) \left(\frac{T+273}{100} \right)^3$$

ρ = emissivity of the solid surface

$\beta = 1$, $\gamma = \frac{2}{3}$ in most practical situations

ϕ is given by a graph in Kunii and Smith (60)

This equation was also quoted by Yagi and Kunii (59) who showed that the fit was better than 20% for most experimental data.

The graphs of Yagi and Kunii (61,62) and Hill and Wilhelm (63), show that the variations of the stagnant conductivity term k_e^0/k_g due to radiation effects is negligible over the temperature range 340-440°C for non-metallic particles. Using the equation derived by Kunii and Smith and assuming a solid emissivity $\rho = 0.75$, recommended by Kunii and Furusawa (64), $k_e^0/k_g = 8.0$. This compares favourably with the literature values in fig 2.1, of around 10.0 for non-metallic packing. The work of Gros and Bugarel (65) differs greatly, as they experimentally obtained a very high conductivity and a very low heat transfer coefficient. This is due to the very high degree of correlation between these two parameters when they are calculated from the same experimental data. Ignoring the work of Gros and Bugarel ϕ (the slope of the lines) in fig 2.1 varies from 0.061 to 0.136 with 0.10 being an average value.

Yagi and Kunii (62) and Olbrich and Potter (66) both obtained values of ϕ for glass spheres for various diameter ratios (D_p/D_t) (see fig 2.2) showing that the fluid flow contribution decreases for increasing diameter ratio. Yagi and Kunii show that this effect is more important for cylinders and rashig rings, for which most of the literature correlations have been produced, and that the absolute value of ϕ for spheres is less than for cylinders and other shapes. Olbrich and Potter obtained their conductivity correlations by assuming a very high value of the modified Biot number ($h_w d_p/k_e = 2.12$) so their overall effective conductivity correlations are doubtful; however the effect of D_p/D_t should be reasonably accurate and does compare favourably with Yagi and Kunii's results.

Extrapolating both Yagi and Kunii's and Olbrich and Potter's data in fig 2.2 to a particle to tube diameter ratio of 0.268, gives a value of 0.053 for ϕ . Assuming the contribution of the stagnant conductivity term to be 10, the derived final correlation to use for the radial effective conductivity is

$$\frac{k_e}{k_g} = 10 + 0.053 \text{ Re Pr}$$

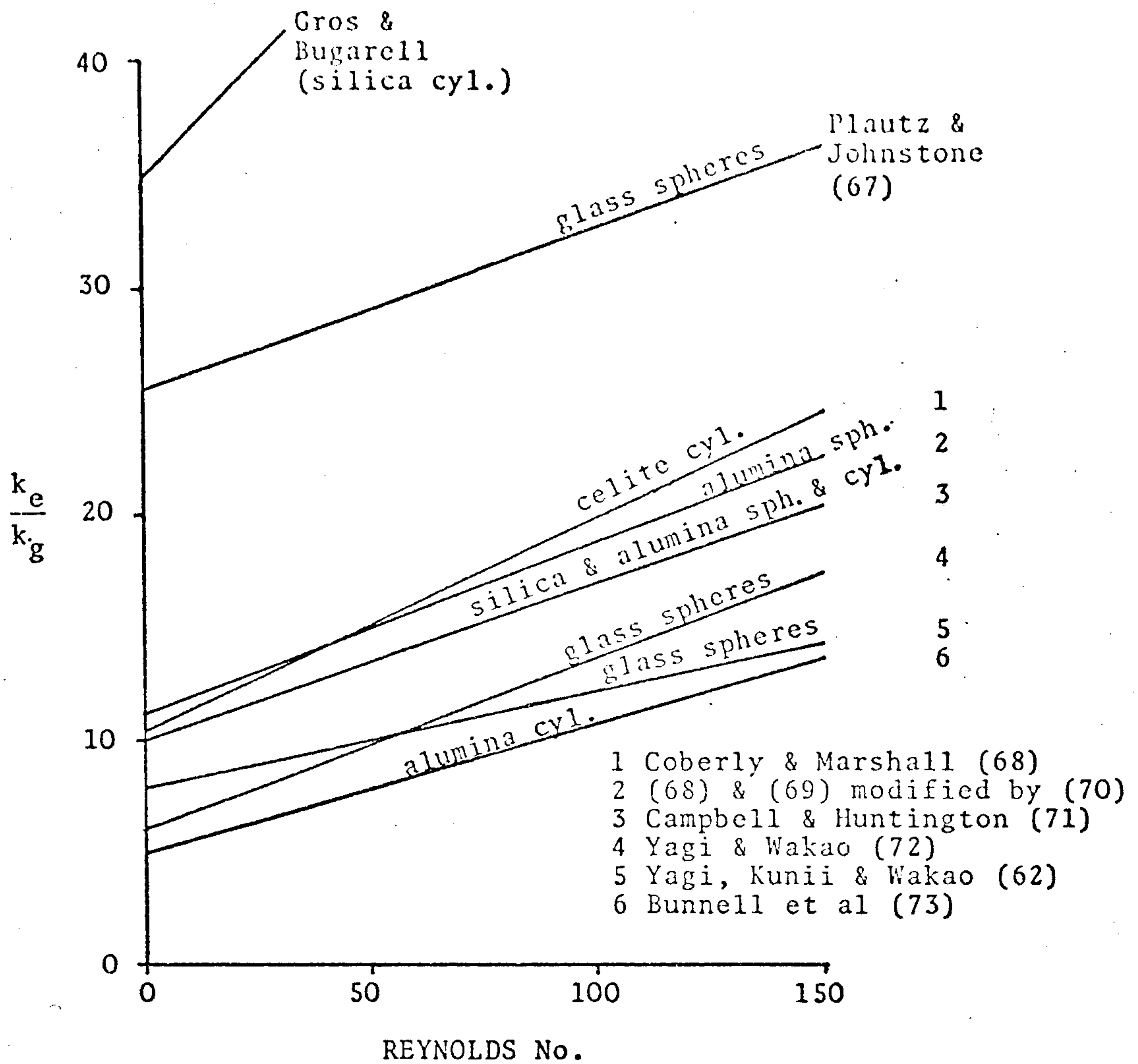


Fig 2.1 EFFECTIVE RADIAL CONDUCTIVITY CORRELATIONS

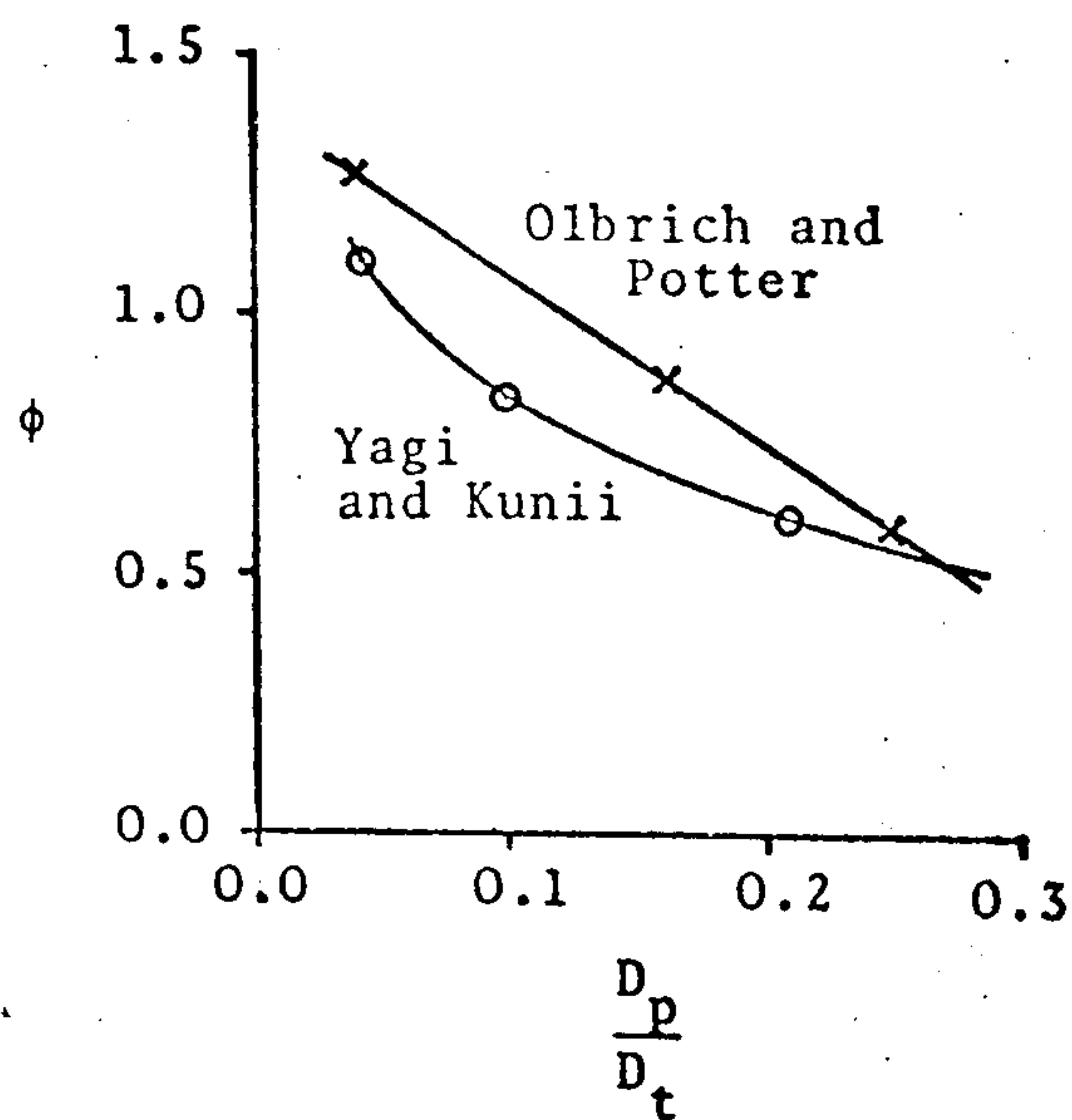


Fig 2.2 ϕ vs DIAMETER RATIO

2.5 Wall Heat Transfer Coefficients

Wall heat transfer coefficients are normally expressed in two ways:

$$Nu = Nu^0 + \lambda Re Pr \quad (1)$$

$$Nu = b Re^c \quad (2)$$

$$\text{where } Nu = \frac{h_w D_p}{k_g}$$

Both forms are equally favoured. The second form initially appears to be the correct form as the Nusselt number should be expected to be zero at a Reynolds number of zero. The effective radial conductivity however is not constant across the whole packed bed but falls off sharply near the tube wall due to the increase in void fraction and the presence of a boundary layer. The increase in the void fraction was reported by Schwartz and Smith (74) and measured by Kimura et al (75). To allow for this effect the decrease in effective radial conductivity near the tube wall is commonly lumped into the wall heat transfer coefficient by adding a stagnant Nusselt number Nu^0 . The radial variation in conductivity decreases with increasing gas flow rate so correlations of the second form are normally only valid at a Reynolds number greater than about 30.

Various correlations for heat transfer coefficients are shown in fig 2.3; as can be seen the scatter is similar to that for the effective thermal conductivity correlations. There is even a large difference between correlations based on the same data but produced by

different workers. The Nusselt number for cylinders is greater than for spheres ignoring the results of Gros and Bugarel mentioned previously, mainly due to the cylinders making better contact with the tube walls than for spheres.

Yagi and Wakao (72) calculated wall heat transfer coefficients from their experimental work with packed beds of spheres and correlated their data along with that of Felix (76) and Plautz and Johnstone (67) by:

$$\text{Nu} = 0.18 \text{ Re}^{0.80} \quad 20 < \text{Re} < 2000$$

Plautz and Johnstone carried out their experiments in a large 0.020m tube with glass spheres of 0.0013 to 0.0019m at Reynolds numbers between 100 and 2000 correlating their data by

$$h_w = 0.090 G^{0.75}$$

which is equivalent to

$$\text{Nu} = 0.273 \text{ Re}^{0.75}$$

Hanratty (77) derived the following correlations for cylinders

$$\text{Nu} = 0.95 \left(\frac{\text{Re}}{\epsilon} \right)^{0.5} \quad 40 < \text{Re} < 240$$

which reduces to

$$\text{Nu} = 1.36 \text{ Re}^{0.5}$$

and also correlated the work of Plautz (78) and Felix (76) for glass spheres at Reynolds numbers between 40 and 1,300 by:

$$\text{Nu} = 0.12 \left(\frac{\text{Re}}{\epsilon} \right)^{0.77}$$

or

$$\text{Nu} = 0.243 \text{ Re}^{0.77}$$

Beck (79), making many assumptions, derived a wall heat transfer correlation for spheres in a packed bed based on Thoenes and Kramers (80) experimental work on mass transfer. At low Reynolds number the equation is numerically identical to Hanratty's correlation of Plautz and Felix's work however the form is very different

$$Nu = 0.203 Re^{\frac{1}{4}} Pr^{\frac{1}{4}} + 0.220 Re^{0.8} Pr^{0.4}$$

Yagi and Kunii (81) re-correlated the results of many workers to the linear form with the stagnant Nusselt term.

Non-metallic spheres:

Yagi and Wakao (72)

$$Nu = 5 + 0.054 Re Pr \quad 100 < Re < 500$$

Felix and Plautz and Johnstone

$$Nu = 8 + 0.054 Re Pr \quad 100 < Re < 2000$$

Non-metallic cylinders

Coberly and Marshall (68)

$$Nu = 20 + 0.069 Re Pr \quad 80 < Re < 2000$$

The coefficient λ of the $RePr$ group was found to be 0.054 in most cases. Fig 2.3 shows these correlations for the largest values of the diameter ratio studied. Yagi and Kunii reasoned that in cylindrical packed beds at low Reynolds number, the radial temperature distribution approached the constant wall temperature leading to inaccurate measurements. They carried out their experiments in an annular bed packed with spheres, with steam and water as the heat transfer fluids to provide an easily measured radial temperature profile. The constant λ in the fluid flow term of equation (1) was found to be 0.041 and not 0.054 which was attributed to the

difference in the packing states of cylindrical and annular packed beds. Fig 2.4 shows the large variation of the stagnant Nusselt number that was found for different diameter ratios. No reliable data is available at all for diameter ratios greater than 0.15.

Leva and co-workers (82,83,84) produced correlations for the overall heat transfer coefficient, where the wall heat transfer coefficient and the effective radial thermal conductivity are lumped into one parameter. Consequently this value is lower than the wall heat transfer coefficient by itself. Leva (85) developed correlations at diameter ratios greater than 0.35, and found that the overall heat transfer coefficient was much larger than expected when extrapolated from his original correlations at low diameter ratios. He postulated that this was due to the channelling caused by the wall effect in such systems.

Due to the large variations of the correlations and accepting the trend in fig 2.4 for non-metallic spheres, the best overall correlation for the present study is to assume the highest reasonable value of the Nusselt number correlations for spheres, namely the modified form of Plautz and Johnson's results produced by Yagi and Kunii.

$$Nu = 8 + 0.054 Re Pr$$

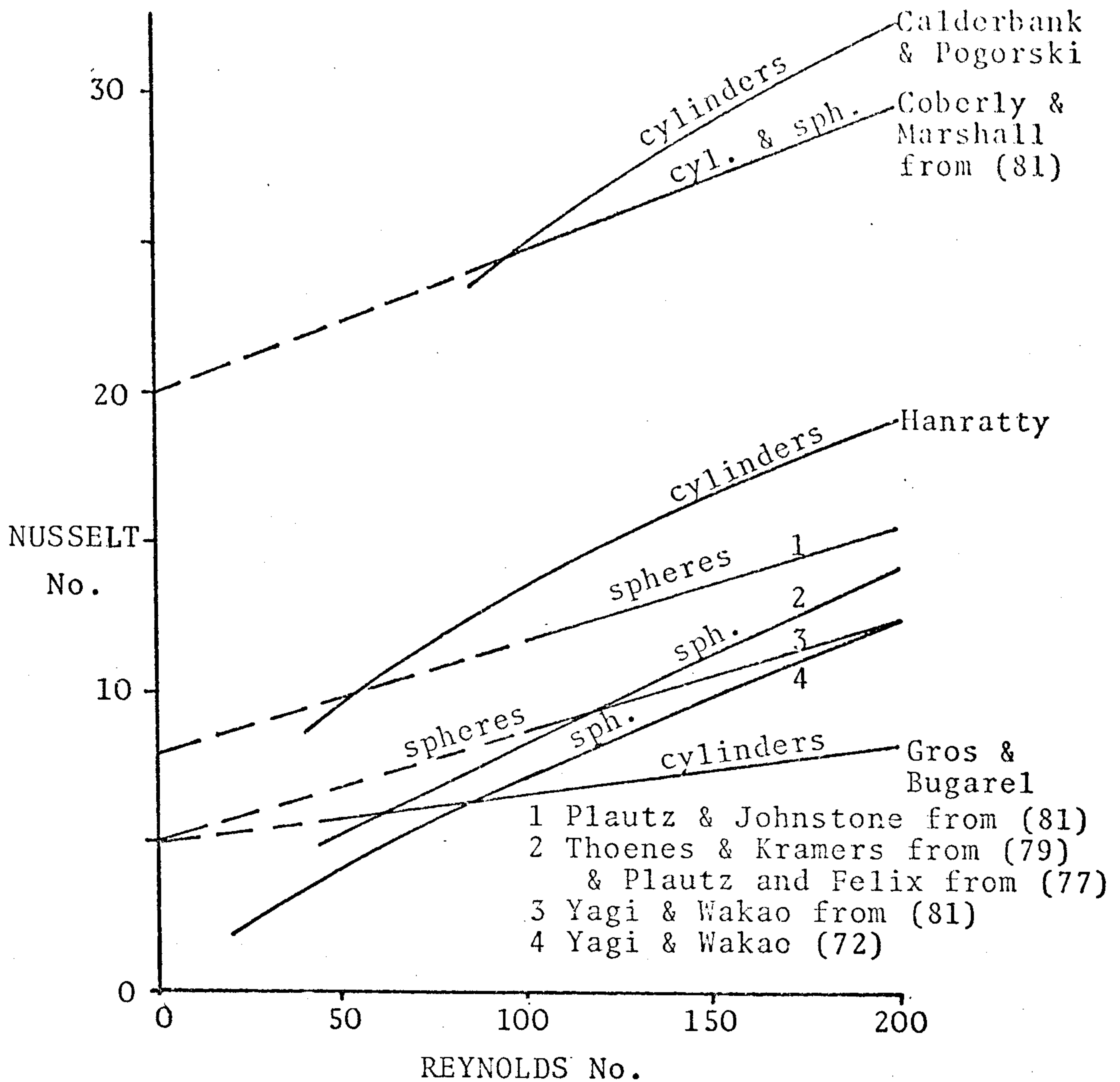


Fig 2.3 WALL HEAT TRANSFER COEFFICIENTS

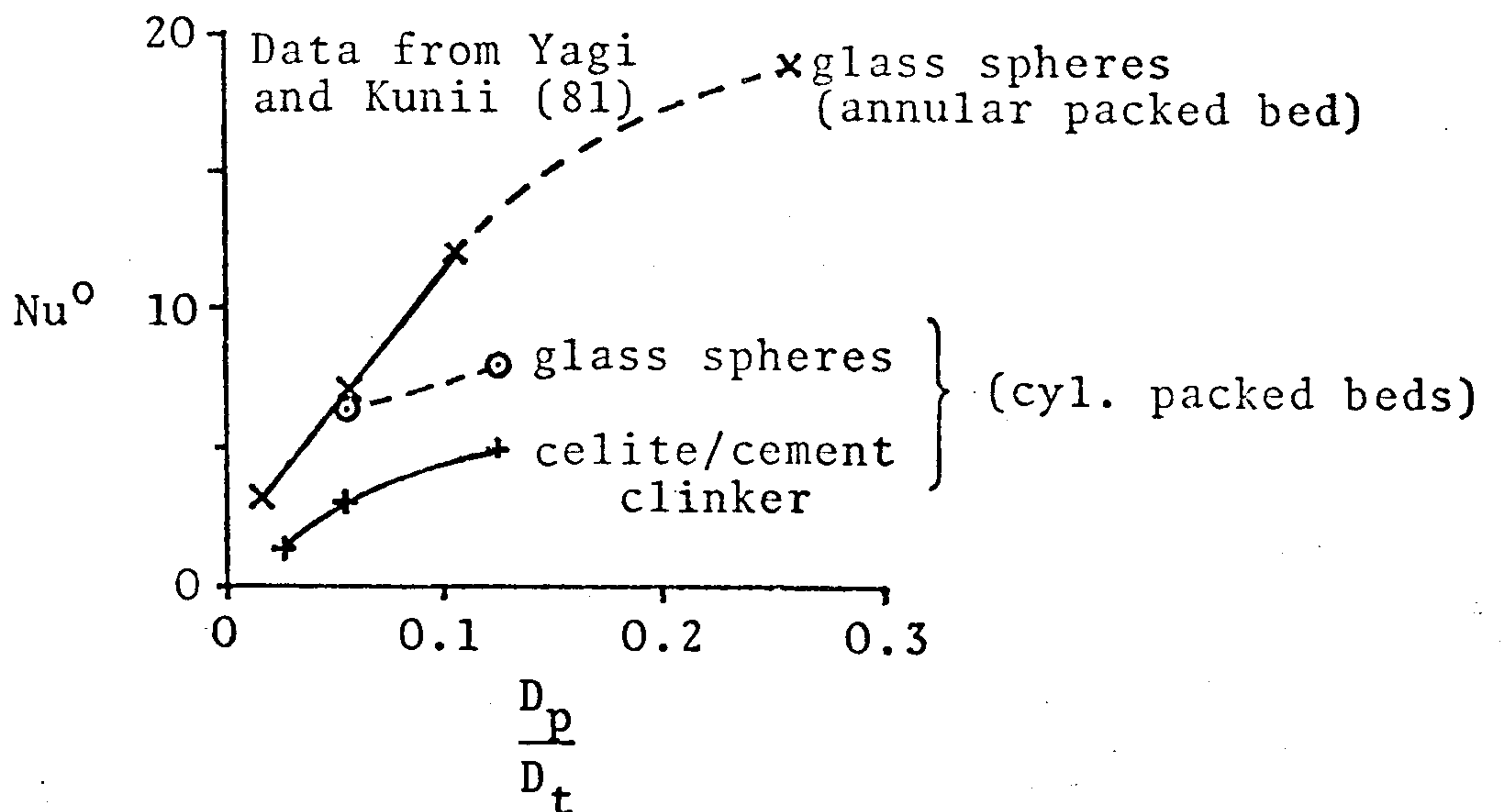


Fig 2.4 STAGNANT NUSSELT No. vs DIAMETER RATIO

2.6 Particle Heat and Mass Transfer Correlations

Most heat and mass transfer correlations produced have been of the Chilton-Colburn j factor form

$$j_d \text{ or } j_h = a \text{ Re}^{-b}$$

where

$$j_d = \frac{K_G}{u} \text{Sc}^{\frac{1}{3}} \qquad j_h = \frac{h_p}{C_p G} \text{Pr}^{\frac{1}{3}}$$

and the particle Reynolds number $\text{Re} = G D_p / \mu$

Carberry (86) carried out a theoretical derivation from boundary layer theory to obtain

$$\epsilon j_d = 1.15 \left(\frac{\text{Re}}{\epsilon} \right)^{-\frac{1}{2}}$$

or

$$j_d = 1.65 \text{ Re}^{-\frac{1}{2}} \qquad 0.5 < \text{Re} < 500$$

where $\epsilon = 0.488$ the void fraction of the reactor.

Carberry and White (87) used this expression for both the heat and mass transfer coefficients in their reactor model.

Pfeffer and Happel (88) derived analytically, heat and mass transfer correlations from the energy equation based on the free surface model for $\text{Re} < 100$

$$j_h = j_d = 3.0 \text{ Re}^{-\frac{1}{2}}$$

Bradshaw and Bennett (89) calculated two mass transfer correlations experimentally from air flowing through a bed of naphthalene pellets, the first without allowing for axial mixing,

$$j_d = 0.506 \text{ Re}^{-0.293} \quad 400 < \text{Re} < 100000$$

and the second corrected for axial mixing.

$$j_d = 0.606 \text{ Re}^{-0.309} \quad 400 < \text{Re} < 100000$$

The difference between the two curves is less than 8% and can be ignored for high Reynolds numbers. Bradshaw and Bennett corrected for axial mixing, the experimental work of Hobson and Thodos (90) and Chu et al. (91), who worked in the particle Reynolds number ranges 40-350 and 200-1300 respectively. In both cases the difference is much greater, up to 16%, showing that in the short packed beds used in these experiments, axial dispersion is important at low Reynolds numbers and should be considered when selecting correlations. Only j factor correlations therefore for experimental work carried out in long packed beds and/or corrected for axial dispersion have been considered. This eliminates most of the work carried out on heat transfer correlations.

The j factor ratio j_h/j_d is commonly accepted to be close to unity. Values of 1.058 and 1.08 were reported by M^CConnachie and Thodos (92) and Gamson, Thodos and Hougen (93) respectively for experimental investigations. Gupta and Thodos (94) re-correlated the results of 8 workers for j_d factors and 4 for j_h factors with overall errors of 17% obtained a j factor ratio of 1.076 but as in the previous papers of Thodos mentioned, no corrections were made for axial dispersion. De Acetis and Thodos (95) obtained a j factor ratio of 1.51. Although they did correct their experimental data for axial dispersion, they did not correct

for conduction and radiation effects. As has been shown by previous workers, and from the trend in fig 2.5, the heat transfer j factor is slightly larger than the mass transfer j factor, so that a j factor ratio of 1.08 would seem appropriate.

M^CCune and Wilhelm (96) , calculating mass transfer rates from 2-naphthol pellets into water flowing in a long packed bed, postulated a correlation for low Reynolds numbers almost identical to that obtained by Carberry

$$j_d = 1.625 \text{ Re}^{-0.507} \quad \text{Re} < 120$$

$$j_d = 0.687 \text{ Re}^{-0.327} \quad \text{Re} > 120$$

Glaser and Thodos (97) using solid metallic particles heated electrically in a long packed bed derived the heat transfer j factor correlation:

$$\frac{j_h}{j_{h_o}} = 1 + \frac{\sqrt{A_p}}{D} \log \frac{4984.}{\text{Re}_h^{0.933}} \quad 30. < \text{Re} < 2700$$

where

$$j_{h_o} = \frac{0.535}{\text{Re}_h^{0.30} - 1.6}$$

$$\text{Re}_h = \frac{\sqrt{A_p} G}{\mu (1-\epsilon) \phi}$$

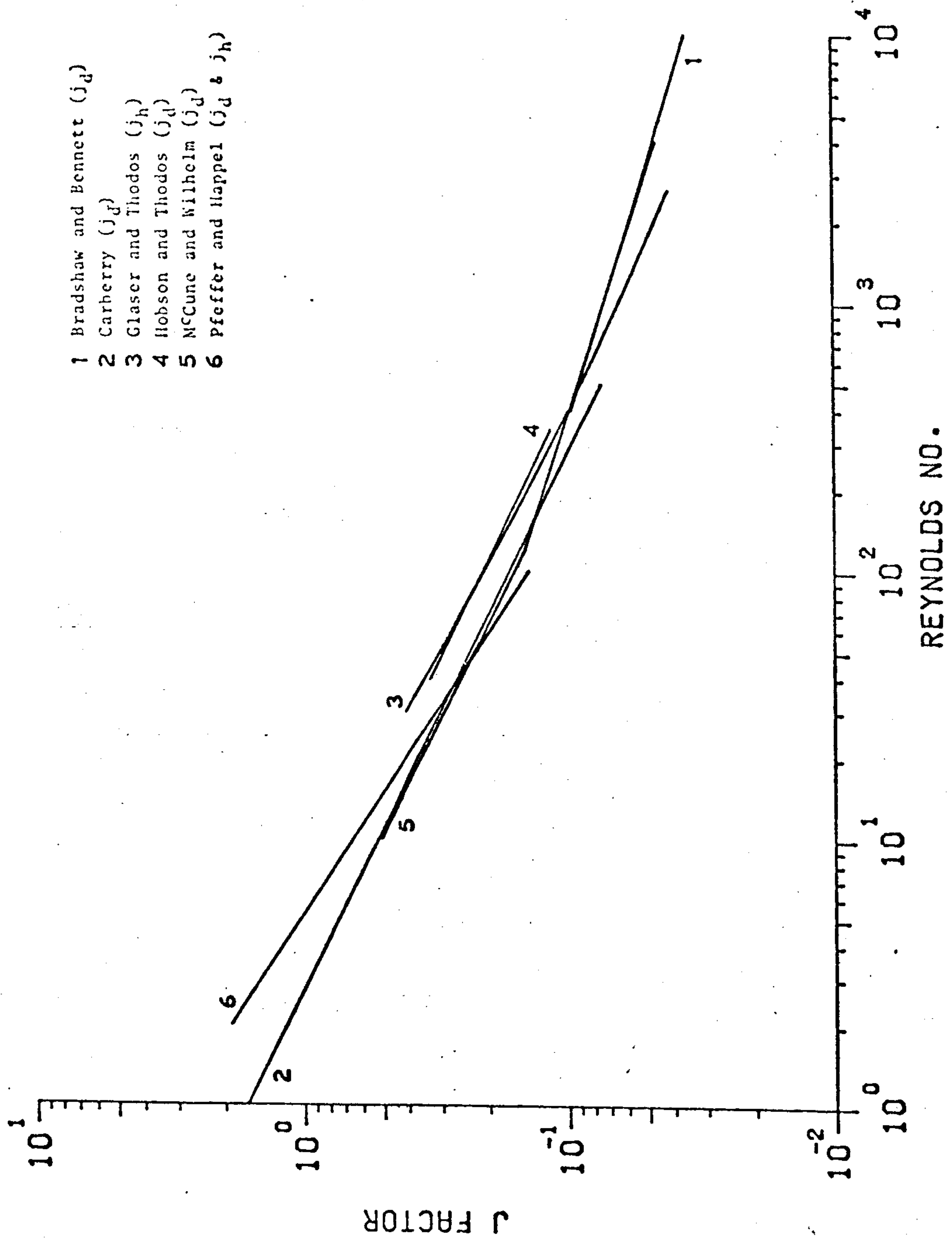
$$\equiv \frac{\sqrt{\pi}}{(1-\epsilon)} \text{ Re}$$

A_p = surface area of 1 particle

D = tube diameter

ϕ = sphericity factor, 1 for spheres.

Fig 2.5 FILM HEAT AND MASS TRANSFER COEFFICIENTS



Most of the experimental work carried out has been at a bed porosity of 0.40 with a diameter ratio less than 0.16. Of the correlations selected only Carberry and Glaser and Thodos have included bed porosity as a parameter. The effect of increasing the bed porosity from 0.40 to 0.488, the value used for this study, is according to Carberry's correlation to decrease the j factor by 11%. To estimate the mass transfer j factor therefore, take the lowest curve in fig 2.5 for the required Reynolds number.

2.7 Effective Radial Diffusivity

When a packed bed catalytic reactor is non-isothermal and non-adiabatic, all of the parameters reviewed may be important. The effective radial diffusivity of mass however, can vary over a wide range (1) with very little effect on the axial and radial temperature profiles. Normally the effective radial diffusivity is correlated by the Peclet number being equal to constant. Froment (2) recommends that the Peclet number should be between 8 and 11. A value of 8 has been used in this study due to the high catalyst pellet diameter to tube diameter ratio.

Chapter 3EXPERIMENTAL METHOD

All experimental work, except for a few calibrations and the light gas analyses, was carried out on the equipment shown in fig 3.1.

Supply of Reactants

Air supplied from a compressed air cylinder was metered through a rotameter before entering the pre-heating serpentine. To keep the catalyst active the reactant stream should contain 0.01 mole% sulphur. This was added to the air stream by metering 99% purity sulphur dioxide, from a gas cylinder, through a water bubbler.

The reagent grade o-xylene (99% pure) supplied by BDH was delivered by gravity feed from a reservoir through a capillary and a Hoke micro-metering valve to the pre-heating serpentine where it flowed down the tube wall and evaporated into the air stream. The glass capillary (approximately 0.3 mm I.D. x 150 mm) was necessary to restrict the o-xylene flow in order to increase the region of useful control of the micro-metering valve. Fine control was by the micro-metering valve, while coarse control, over a limited range, was effected by varying the liquid head in the reservoir. A burette was connected to the reservoir so that by closing the reservoir stopcock the o-xylene flow rate could be measured by timing the decreasing level in the burette. Due to the large surface area of the reservoir

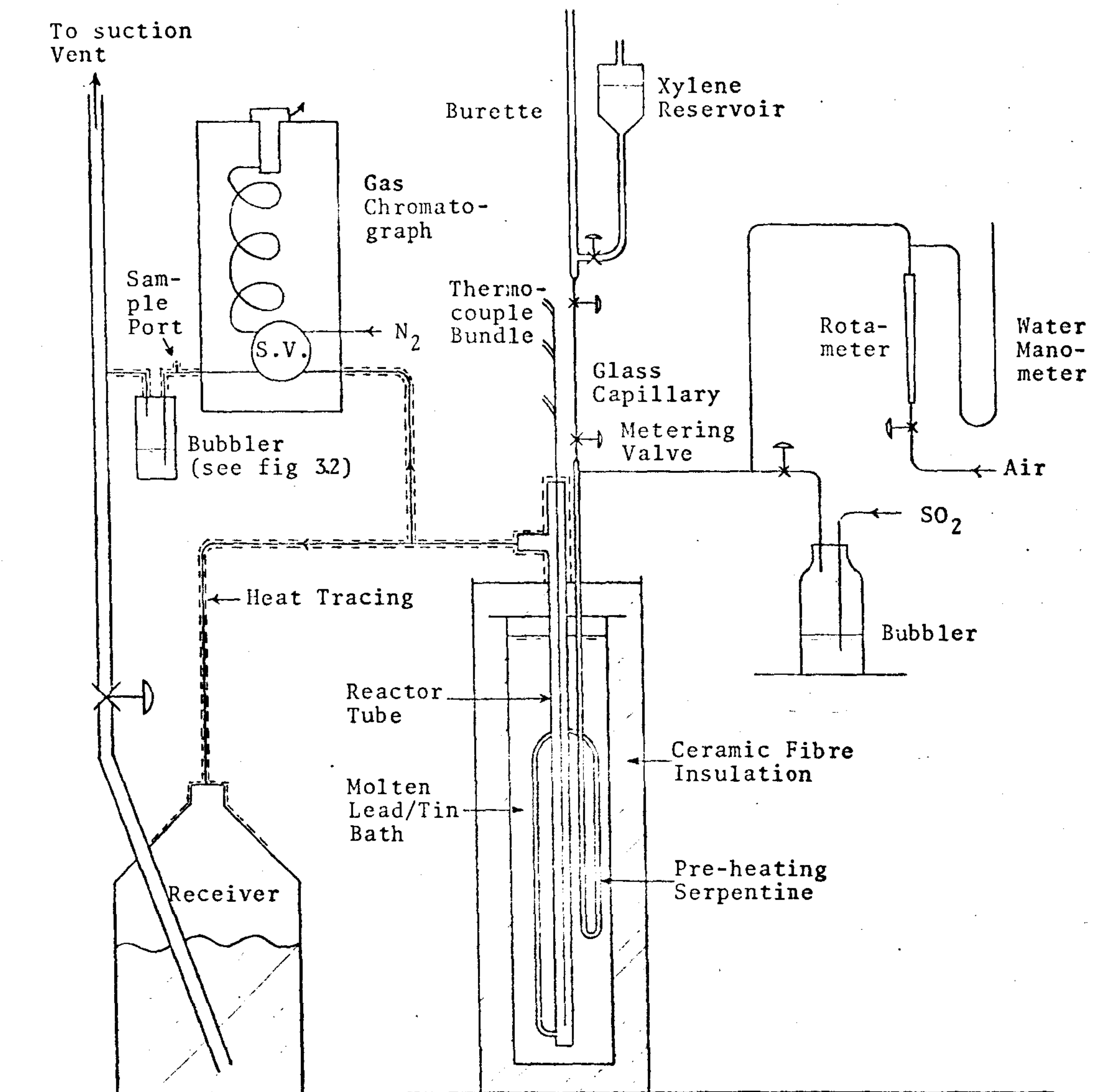


Fig 3.1 EXPERIMENTAL APPARATUS

and the very low flow rate (10mls/hr o-xylene into 480 l/hr air = 0.41 mole%) the liquid head decreased only very slowly during a run and could be topped up occasionally to maintain a constant flow rate. Reproducibility and accuracy during a run were better than 2%.

Various positive displacement metering pumps were tried to feed the o-xylene, with a hydraulic accumulator to dampen any flow oscillations, however no smooth reproducible flow rates were achieved, possibly due to the flow rate being at the lower operating limit of the smallest pumps available.

Evaporation of o-xylene into the air stream was not considered due to the sensitivity of the vapour pressure to temperature changes, and the difficulty in producing a step change in the o-xylene concentration while maintaining a constant air flow rate.

Reactor

The pre-heating serpentine (12.7mm O.D. stainless steel) with a heated length of 1.20m, connects directly to the vertical reactor tube (15.59mm I.D. stainless steel) just below a mesh support for the 0.499m of 4.16mm diameter spherical catalyst pellets supplied by von Heyden of Munich, Germany. Both tubes were immersed in the lead/tin solder bath contained in a 0.102m I.D. x 0.610m mild steel tube closed at the bottom and flanged at the top. This was heated electrically and insulated by alumina cement and ceramic fibre.

To determine the reactor temperature, 10 evenly spaced thermocouples were placed axially with the pairs of wires passing up through the bed and out the sealed end of the reactor tube (see fig 3.1). An 11th. thermocouple was implanted in a catalyst pellet at a dimensionless length of 0.222 (0.111m) from the inlet. To drill a hole in the core of the silica catalyst support for insertion of the thermocouple, an ultra-sonic drill had to be used. Unfortunately as much as 20% of the surface area may have been damaged, and as water had to be used in the drilling process, some of the active catalytic species, especially potassium sulphate, may have been removed.

The voltage, relative to the ambient temperature, across the thermocouples was measured by a Solartron data logger with paper tape output capable of scanning eight channels per second. The ambient temperature correction was determined both from a thermocouple in melting ice and by a normal glass thermometer which agreed very well. The thermocouples were Chromel/Alumel with each 0.10mm wire insulated by threading through a glass capillary of approximately 0.23mm O.D. The thermocouples were assembled so that each temperature measuring weld was on the surface of the bundle which was held together, at about 3cm intervals by alumina cement. The thermocouples, although fairly flexible, were kept axial during the packing by the use of a centralising jig that was removed as the catalyst was tapped into place. Unfortunately the first thermocouple

in the bed at a dimensionless length of 0.111 (0.056m) was unknowingly damaged and ceased to function. At the outlet of the catalytic bed the outside diameter of the thermocouple bundle was 1.5mm, or 1% of the cross-sectional area, but for most of the length, the area occupied by the thermocouples was even less. This decreased by 7% the overall packing density from a trial value of 1.42gm/cm³ to 1.33gm/cm³. The reactor however was now changed from a cylindrical to an annular type with less than 2 catalyst pellets across the annulus which may result in channelling of the gas.

In initial trials, stainless steel sheathed thermocouples were inserted radially into the centre of the reactor tube however, not even 80/20 gold/nickel solder could withstand leaching by the lead/tin bath.

All the product lines from the reactor were heated to 180-200°C by Electrothermal heating tape to prevent blockage by condensation of any products, especially phthalic anhydride itself. A side stream was directed for gas chromatographic analysis before the receiver, which was packed with cotton waste.

Heavy Gas Analysis

The sample was introduced into a flame ionisation detection chromatograph by a Taylor Servomex air actuated gas sampling valve, of sample volume 0.679ml, operated from a 30 psig. supply by a manual flow reversing valve. The gas flow through the sample valve was observed via

the bubbler, the final design of which is shown in fig 3.2. The sample valve was contained in the chromatograph oven at 180-190°C. The oven was manually controlled by a Regavolt variable voltage transformer. Temperature stability was $\pm 2^\circ\text{C}$. which is adequate for a flame ionisation detector. A sample port was provided for liquid phase syringe injections. The column (6.35mm O.D. x 0.8m) was 10% XE 60 silica gum on 100-120 mesh diatomite CQ supplied by Pye Unicam. The gas rates were nitrogen carrier gas 66 ml/min., hydrogen 34 ml/min., and combustion air 300 ml/min.

The detector and amplifier, supplied by Pye Unicam had a maximum useable sensitivity of about 2×10^{-6} gm mole/l (1 ppm). The detector and injection port were kept at 265 and 240°C respectively, each being controlled manually by a Regavolt variable voltage transformer.

Calibrations up to 0.3 mole% were carried out by subliming phthalic anhydride into a nitrogen stream at a known constant temperature from which the vapour pressure could be calculated by the following expression developed by Crooks and Feetham (98) for the solid phase up to 130°C.

$$\log_{10} P_{\text{mm}} = 12.249 - \frac{4632.}{T} \quad (T = ^\circ\text{K})$$

Saturation of the phthalic anhydride vapour stream was checked by varying the nitrogen flow rate. The vapour stream was then admitted through heated lines to the gas sampling valve and the gas chromatograph for analysis. For calibrations above 0.3 mole% the calibration was

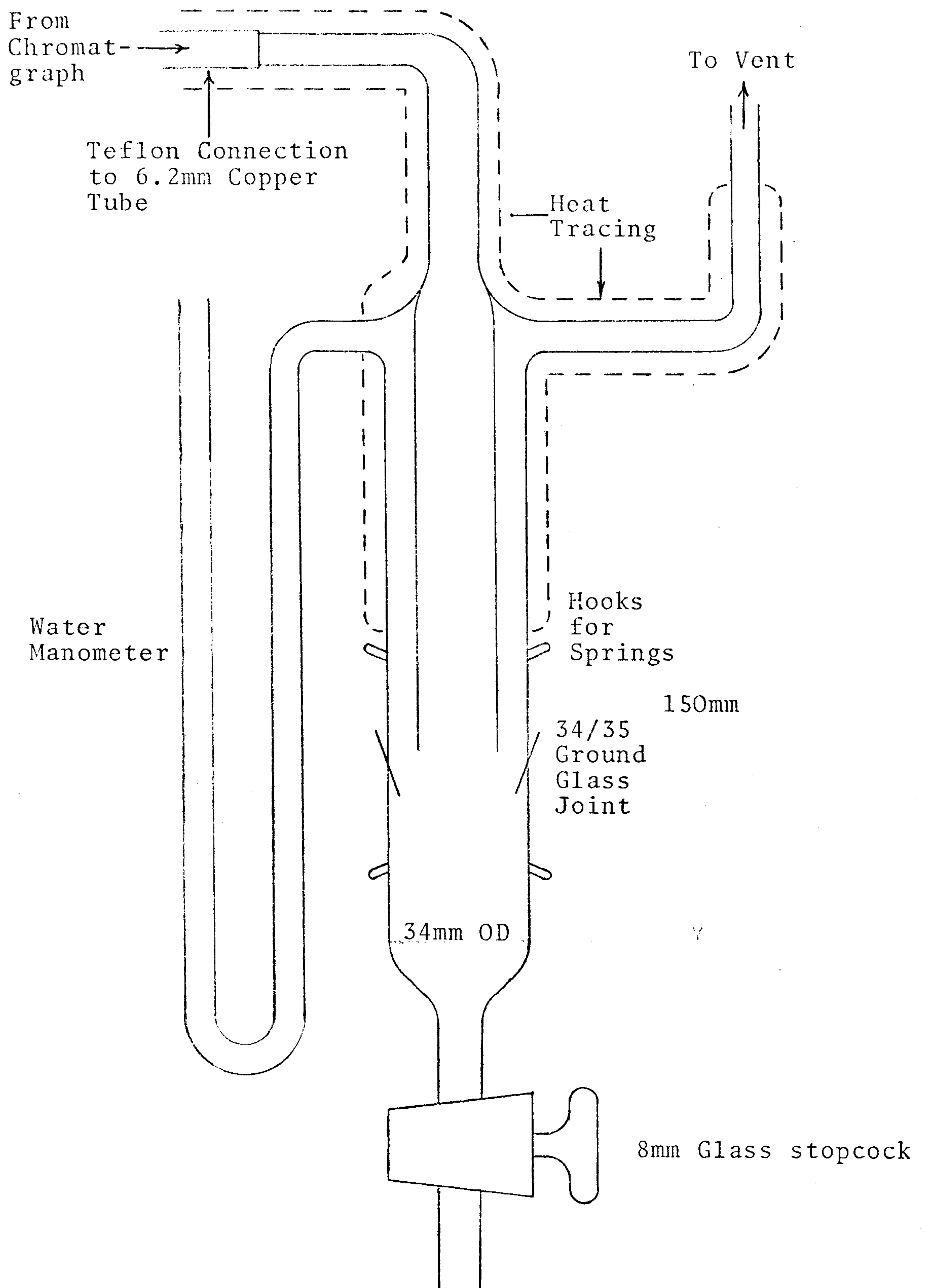


Fig 3.2. Bubbler on outlet of gas chromatograph

linearly extrapolated, as this was still within the linear range of the gas chromatograph. The elution times are shown in table 3.1. Unfortunately the maleic anhydride and o-tolualdehyde peaks could not be separated. At the exit of the gas sampling valve a septum was installed so that when the valve was in its normal by-pass position a sample could be withdrawn for analysis of the light gas components in a second gas chromatograph.

Light Gas Analysis

The utilisation of a second chromatograph was necessary to check the overall mass balance and to determine the CO/CO_2 ratio which is vital when calculating the overall heat of reaction due to the large difference in the respective heats of formation. The light gas analysis was carried out by injection into a programmeable Taylor Servomex gas chromatograph with a katharometer detector (see fig 3.3). Due to the total carbon oxides concentration being about 1 mole% or less the chromatograph was operated at ambient temperature to facilitate good resolution of the components.

The first column (4.8mm I.D. x 1.5m. 50-80 A.S.T.M. mesh Poropak T) separates the sample into two groups of components. The first group to elute, oxygen, nitrogen and carbon monoxide is directed into the molecular sieve column (4.8mm I.D. x 3.66m, 44-60 B.S. mesh, 13x molecular sieve) for further separation. By switching the hydrogen carrier gas flow the carbon dioxide is eluted directly into the second Poropak column (4.8mm x 3.05m, 50-80

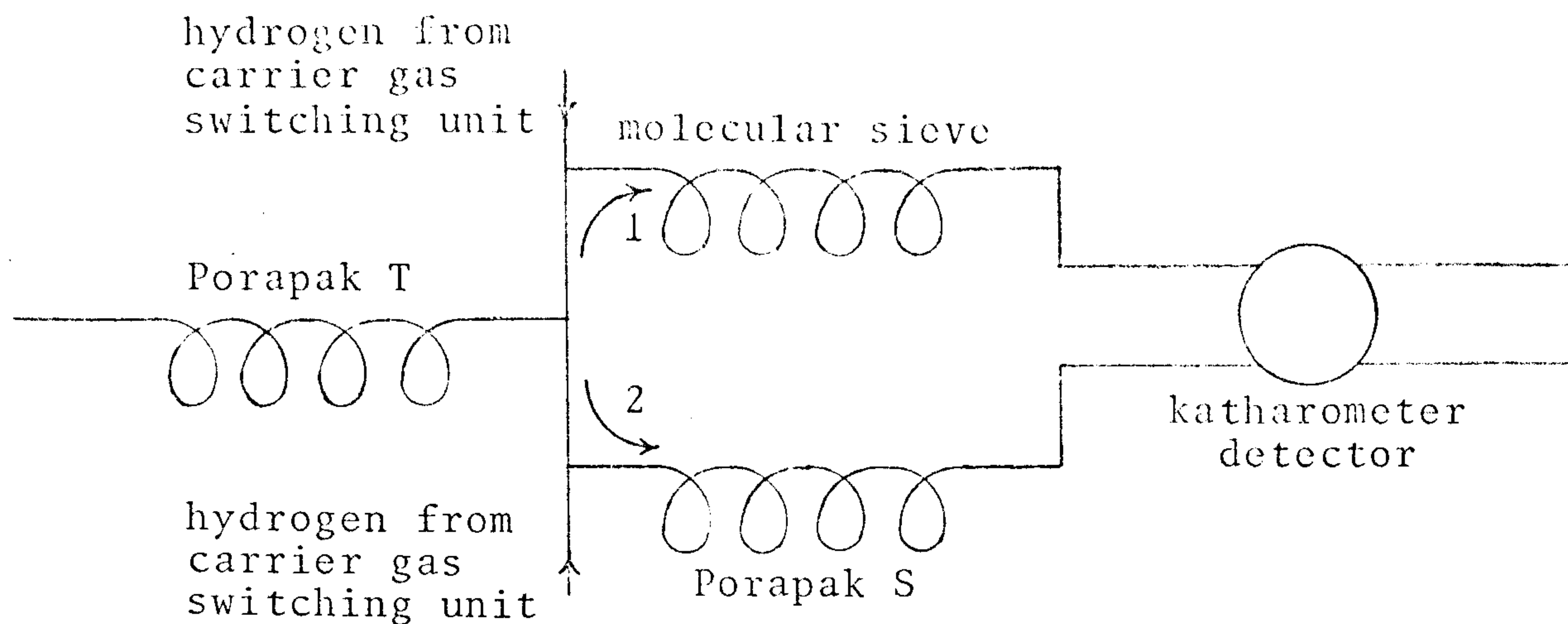


Fig 3.3 GAS CHROMATOGRAPH FOR LIGHT GAS ANALYSIS

Table 3.1 ELUTION TIMES OF HEAVY COMPOUNDS

Compound	Time (s)
o-xylene	35
maleic anhydride	55
o-tolualdehyde	55
citraconic anhydride	60
phthaldialdehyde	110
phthalic anhydride	180
phthalide	200

Table 3.2 KATHAROMETER WEIGHTING FACTORS

oxygen	1.000
nitrogen	0.884
carbon monoxide	0.908
carbon dioxide	1.358

where

$$\text{normalized area} = \frac{\text{area of peak}}{\text{weighting factor}}$$

A.S.T.M. mesh Poropak S), which retards the carbon dioxide until the components of the first group are completely separated. The final elution order is oxygen, nitrogen, carbon monoxide and carbon dioxide. Ideally any heavy components adsorbed on the first Poropak column are removed by back-flushing the column. In practice this was rather ineffective as after 60 minutes of operation, normally four or five samples, no more analysis could be carried out for a further hour while some heavy components eluted, probably o-xylene or maleic anhydride.

Taylor Servomex flow control and switching units were employed to accurately regulate the hydrogen carrier flow, which is critical when using katharometer detectors especially if both arms of the bridge circuit are used as in this case.

Calibrations were performed with 1% certified gas mixtures of carbon oxide supplied by British Oxygen Company. Values obtained for the weighting factors relative to oxygen are shown in Table 3.2.

Immediately after calibration of the flame ionisation chromatograph the overall mass balances were within $\pm 5\%$; however in later runs the error was up to $+ 20\%$ even though temperatures and gas flow rates were kept as constant as was possible. The calibration of the katharometer detector chromatograph did not vary, with reproducibility of analysis being within 2%, so that this analysis was assumed to be absolute and the

total heavy product concentration was determined by difference. The various heavy component concentrations were determined from normalising the area of the respective peaks relative to the total area of the heavy product peaks. For all gas chromatographic analysis, a Vitraton 400 chart recorder with integrator was used.

Operational Procedure

The vanadia catalyst was activated overnight by passing 150 l/hr of air containing 0.01 mole% sulphur dioxide through the reactor.

After setting the air rate at the desired value, the reaction was initiated by gradually opening the micro-metering valve to increase the o-xylene flow rate until this reached the required value. As the reactor approached the desired operating conditions from start-up the power input to the bath was gradually decreased as more heat was evolved by the reaction. To obtain steady state, the power input had to be very carefully adjusted, while monitoring the hot spot thermocouples, as these were very sensitive to changes in the bath temperature. For the last half of the experimental runs, where higher o-xylene concentrations were used, a cooling tube in the reactor bath through which air from a 70psig supply was passed, was used as well as the Regavolt variable voltage transformer to control the bath temperature. The air cooling tube gave a faster response and finer control than controlling the bath temperature by the transformer.

As steady state was approached the o-xylene flow rate was measured and at steady state the gas chromatographic analyses were completed. The valve at the outlet of the receiver being adjusted when necessary to keep a small, but constant flow of gas through the sample valve, observed by the bubbler.

To initiate a step change transient either the o-xylene flow rate or the air rate could be changed. The bath and inlet temperature however, could not be changed step-wise, due to the large thermal mass of the bath. As the o-xylene flow rate was dependent on the head of liquid plus the difference between atmospheric pressure and the gas pressure in the serpentine, changing the air rate altered the pressure drop across the system, resulting in a change in the o-xylene flow rate as well. Changing the o-xylene flow rate, however did not effect the air rate. As the heat evolved in the reactor changed after introducing a transient, the power input to the bath had to be varied by a corresponding amount, so that this feed forward control could keep the reactor bath at a constant temperature.

As a transient was initiated the scanning rate of the data logger, after the first few runs listed, was increased from scanning all the thermocouples every minute, to every five seconds. After about four minutes the scanning rate was returned to normal.

The pressure at the inlet of the system was normally

kept at about 35cm of water (0.5psig) with a careful watch being kept on this in case of tube blockages, possibly due to failure of the heat tracing. The gas flow rate was corrected to 25°C and 1 atm by temperature calculations and a rotameter calibration carried out at the operating pressure, by water displacement in a large inverted measuring cylinder.

The system was seldom completely leak proof, however the leakage rate when the whole system was pressurised to 55cm of water (0.8psig) was kept below 0.2 l/hr, or less than 0.05% of the total flow rate. In actual fact the operating leakage rate was lower than this as the pressure of the system, especially after the reactor, was appreciably lower than the test pressure due to the suction vent line pressure of -5cm of water.

When not in use the reactor was kept at about 270°C with a small flow of air passing over the catalyst at all times.

4.1 Experimental Conditions

Many trial experimental runs were carried out to minimise the operating problems of the system. These were mainly due to non-reproducible results from the flame ionisation detector chromatograph, blockage of the bubbler by the phthalic anhydride in the off gas from the chromatograph, failure of the heat tracing of the product lines and instability of the bath temperature at steady state and especially under dynamic conditions. Elimination of the chromatograph problems are mentioned in chapter 3. Heating tape failures occurred initially, but seldom in the later experiments, while stability of the bath temperature at steady state was achieved through operating experience. For dynamic conditions, where the inlet o-xylene concentration only was varied, manual feed forward control of the reactor bath heating was effectively utilised so that the inlet gas temperature to the reactor normally remained completely constant.

The outside wall temperature of the reactor was measured by a moveable thermocouple probe. The temperature profile is shown in appendix VIII. The maximum variation over the length of the reactor was 3°C. This curve was fitted by a fifth order polynomial and included as the boundary conditions for the partial differential energy equations.

The temperature reading of the thermocouple probe and the two thermocouples in the reactor varied by $\pm 0.5^{\circ}\text{C}$ over

a one minute interval. This was due to the variable nature of the convective circulation of the liquid metal in the bath. The measured centre line temperature of the reactor varied by up to 1°C at steady state, which is very little considering the sensitivity of the reactor temperature profiles to variation of the bath temperature. The variation of the wall temperature, would only be over a small area at a time and appeared to be completely random, as would be expected, so that the overall effect of this would be fairly minor, as found. At very high concentrations and hence high hot spot temperature it was very difficult to obtain a stable operating state. In these cases the random variation of the wall temperature may have been significant and it would be doubtful if even the best automatic control could achieve a steady state. The best solution to this problem would be to have forced convection of the heat transfer medium. This could be achieved by using a fluidised bed or a molten salt bath with pumping, mechanical agitation, or the injection of nitrogen or air as is done in large scale operations. Nevertheless, some variation in the hot spot can be expected due to parametric sensitivity.

For the dynamic condition of a step change in the gas flow rate it was not possible to keep the inlet gas temperature to the reactor constant, by the application of feed forward control. For an increase in the total gas flow rate the inlet gas temperature to the reactor increased by 0.2 to 0.5°C . This is contrary to normal heat transfer theory as at the end of a heated tube the outlet gas temperature should be lower, the higher the flow rate. This can be explained by the pre-heating serpentine acting as both a

heater and a cooler. From appendix VIII it is obvious that the reactor wall temperature, and hence the bath temperature are not constant throughout the molten metal. As shown in fig 3.1 of the equipment design, most of the length of the pre-heating serpentine is in the middle region of the bath. This is the hottest part and due to the length of the pre-heater the gas approaches this temperature. Over the final part of the pre-heater, the bath temperature decreases, so consequently the gas is cooled in this section. By increasing the gas flow rate therefore, less cooling takes place, resulting in the observed slightly higher inlet temperature.

The pellet temperature supposedly measured by a thermocouple inserted in the pellet, never registered a temperature higher than the thermocouple positioned in the centre line. Dynamic response tests were carried out with the catalyst bed initially at a steady state temperature with a very small gas flow rate through the bed. The gas rate was suddenly increased to maximum flow rate, with the temperature response of the thermocouples being recorded at one second intervals. In all of these tests the response of both thermocouples was identical and consistent with a measuring device of very low thermal mass. This shows that the thermocouple had probably come out of the catalyst pellet. In the construction of the thermocouple bundle the glass capillary sheaths were cemented together approximately every 3cm and especially just before each thermocouple to ensure that they were kept as central as possible. The thermocouple inserted in the catalyst pellet however was

only cemented about 4cm from the end to facilitate bending away from the centre line due to the diameter of the pellet. If the pellet came off during the packing process this large free length of the thermocouple could easily then mean that the pellet ended up at, or near the wall of the reactor. Due to the radial temperature profile being approximately parabolic this would result in the thermocouple, supposedly inserted in the catalyst pellet, recording a lower temperature than the centre line thermocouple, as observed experimentally.

Replicate steady state runs were carried out with both the temperature profiles and the outlet concentrations agreeing within experimental error.

4.2 Product Distribution

The yield obtained for the production of phthalic anhydride from o-xylene, as can be seen from the experimental data in appendix VII, was 76-80% or 106-112 Kg phthalic anhydride per 100 Kg o-xylene, which is at the top end of the industrial yield range of 100-110 Kg/Kg. The reactor used was 0.5m in length compared to the industrial units of 3m with a residence time half that of commercial reactors. The difference in residence times would explain the decreased amount of over oxidation observed experimentally.

As the compounds being analysed in the flame ionisation detector chromatograph were not too dissimilar and a quantitative product analysis was not required, a constant weighting factor of unity was used for all compounds. Normally

phthalic anhydride comprised around 97% of the heavy hydrocarbons in the outlet stream so that this assumption is quite reasonable when calculating the phthalic anhydride yield. For the products of the low bath temperature runs however, where up to 34% of the o-xylene feed was left unreacted, this assumption may be very misleading. The phthalic anhydride yield for the low bath temperature runs, calculated by the remainder method normally used, was about 10% in error compared with a calibration for the gas chromatograph based on the results of other runs. This can be corrected if a relative sensitivity for o-xylene to phthalic anhydride of 0.65 is assumed in which case all comparisons of yield from the two methods are within 3%.

The assumption of a non-unity relative sensitivity for o-xylene is only important for the low conversion runs 24 and 29 where it can result in an increase in the phthalic anhydride yield of up to 15%. The results in appendix VII for these runs has been corrected accordingly, however no modelling was carried out based on these data. In the rest of the experimental runs the maximum fraction of unreacted o-xylene was 0.01 so application of the o-xylene relative selectivity would only change the phthalic anhydride yield by a negligible amount (a maximum of 0.3%).

The major by-product, after the carbon oxides, was either o-tolualdehyde or maleic anhydride, but the gas chromatograph could not separate these components. Experimentally the yield of this product increased from 1.5 to 2.0% as the hot spot temperature increased, so that it

was assumed to be maleic anhydride as more over oxidation would be expected to occur at higher reaction temperatures. For the low bath temperature runs however, the yield was up to 6%. This implies that this product may have been o-tolualdehyde as it is commonly quoted as an intermediate in the reaction of o-xylene to phthalic anhydride.

No relative sensitivity other than unity was used for maleic anhydride as normally this was a minor product, and any small change in this would only make a slight change to the phthalic anhydride yield. For the low conversion runs, although the heavy by-product yield was much higher, a unity relative sensitivity was satisfactory as no detailed calculations were intended for this case.

Occasionally, especially at the start of a run, a trace of phthalide was detected, but the poor separation of the phthalic anhydride and phthalide peaks meant that the former completely overshadowed the latter. Normally a trace of citraconic anhydride (methyl maleic anhydride) was detected and possibly pyrocinchonic anhydride (dimethyl maleic anhydride). At normal operating temperatures no phthaldialdehyde was detected; however at low bath temperature runs, hence at low conversion, a trace was detected.

In all of the runs carried out no traces were found of o-toluic acid, benzoic acid or benzoquinone. Occasionally a trace component was detected with an elution time of approximately 12 minutes. This was assumed to be the black deposit that gradually blocked up the product lines

although they were kept at nearly 200°C. Calderbank (99) claims that this compound is the result of the reaction of o-xylene with phthalic anhydride to form a multi-ring compound. Due to the limited operating conditions of the gas chromatograph it was not possible to conclusively identify this substance.

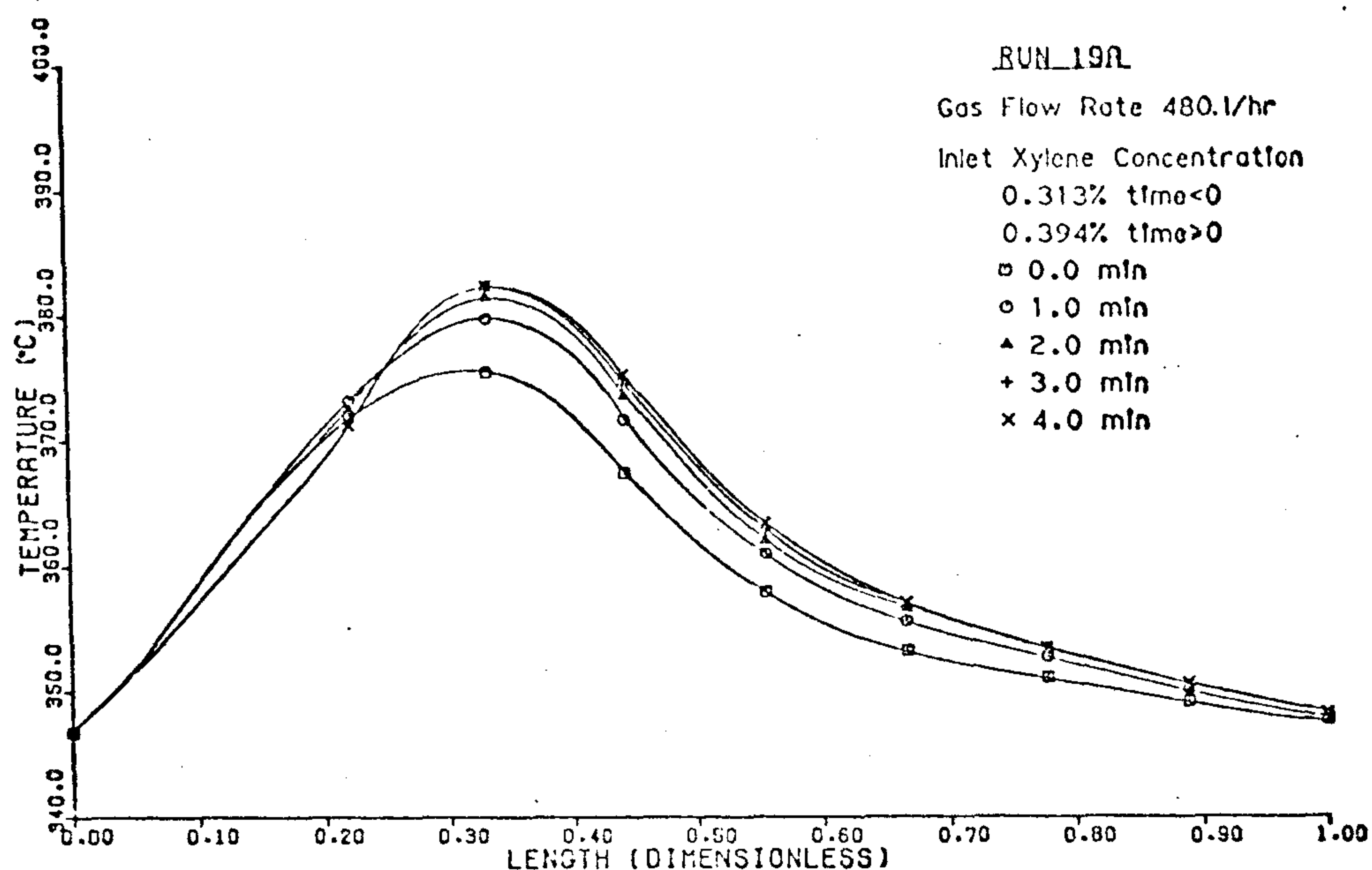
The highest yield obtained of 80% was achieved at low inlet o-xylene concentrations of 0.31 to 0.40 mole%, with hot spot temperatures less than 390°C. Under these conditions the total carbon oxides yield was 18% with a CO_2/CO ratio of approximately 2.75, while the yield of maleic anhydride was 1.5% with the remainder in all cases of about 0.5% unreacted o-xylene. The overall heat of reaction was approximately -1.61×10^6 KJ/Kmole. As the concentration was increased to 0.72% the hot spot temperature increased and the yield of phthalic anhydride decreased to 76%, while the total carbon oxides increased to 21.5% with a CO_2/CO ratio very slightly decreased to 2.6. The yield of maleic anhydride was 2%. Although a lower carbon oxides ratio was obtained, the higher overall degree of oxidation of the products resulted in the heat of reaction changing to -1.70×10^6 KJ/Kmole.

4.3 Wrong Way Behaviour

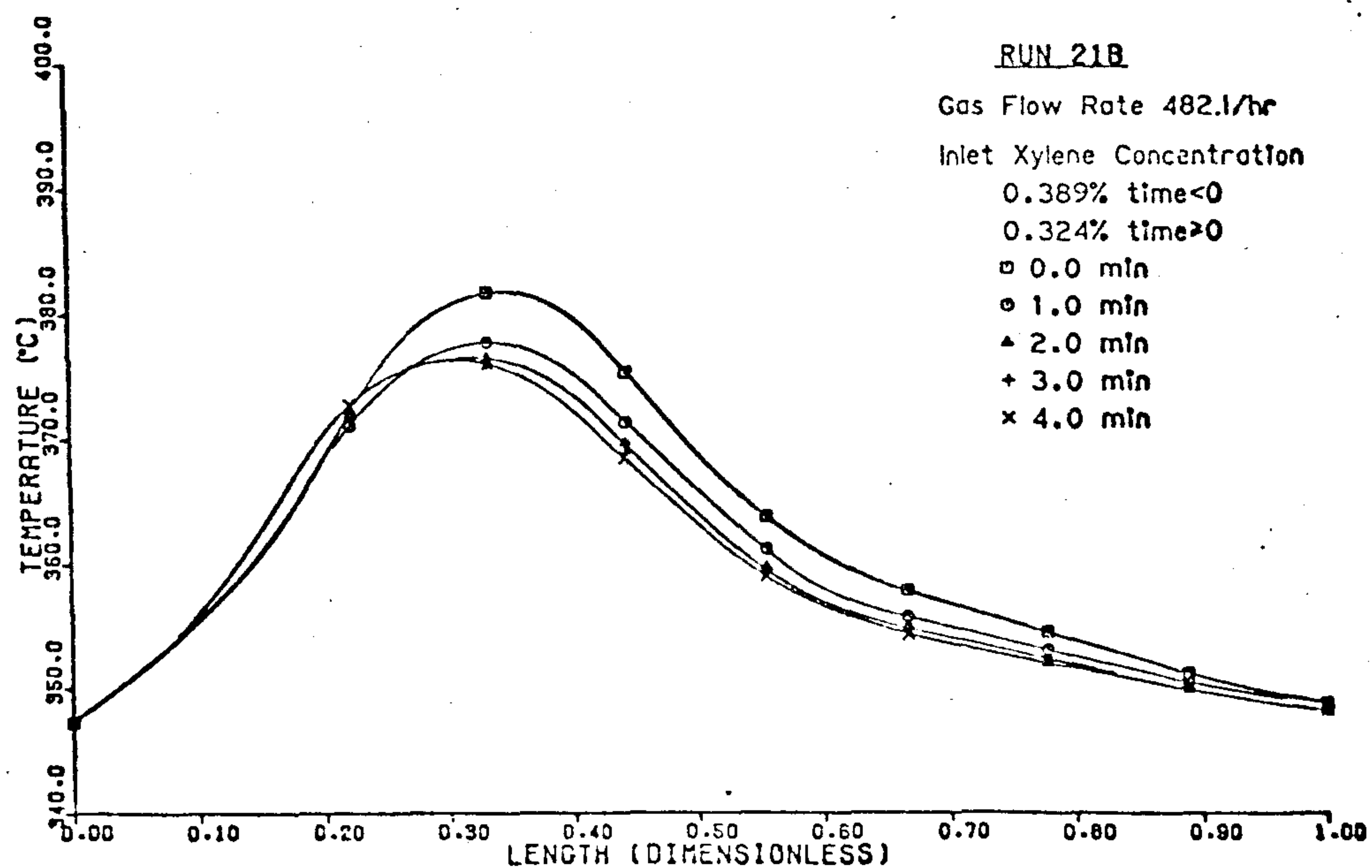
At all bath temperatures studied, in the o-xylene concentration range 0.31 to 0.52 mole%, with a constant air flow rate, an anomolous effect was found. Increasing the o-xylene concentration resulted, for a dimensionless position of 0.222 (0.111m), in an initial small temperature

rise followed by a decrease to a new lower steady state temperature, see graphs 4.1 and 4.3. This temperature decrease, or wrong way behaviour occurs instead of a monotonically rising temperature which would be expected for a normal first order system, at a position before the hot spot. The experimental hot spot moved slightly towards the outlet of the reactor and increased in height, however the movement of the hot spot was in the opposite direction to the movement that would occur in a similar first order reaction system. This effect was completely reversible when the o-xylene concentration was decreased, see graphs 4.2 and 4.4. The second half of the catalytic bed appeared to behave in all cases as if a simple first order reaction was taking place.

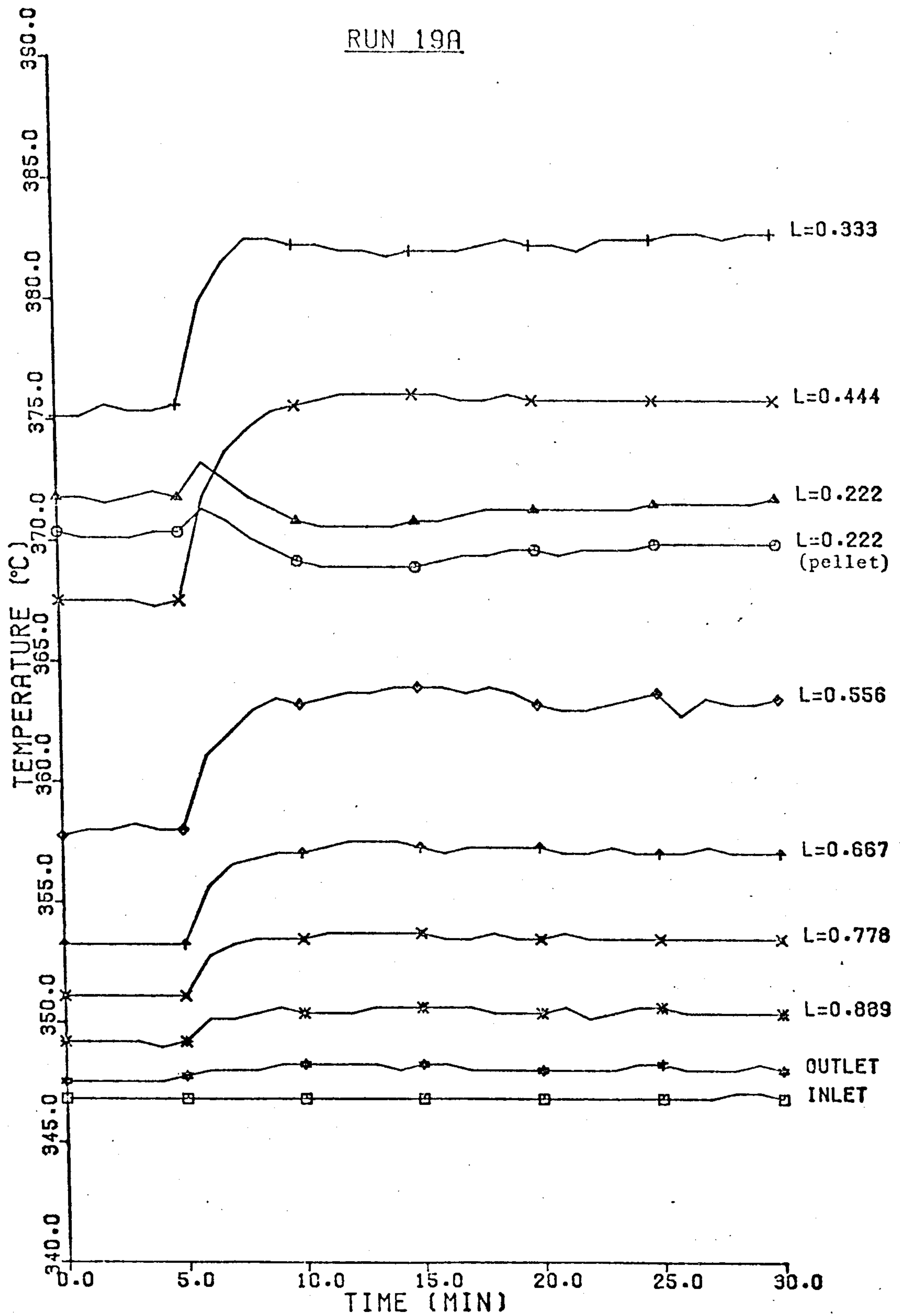
To explain the wrong way behaviour physical factors were first investigated, namely the change in the overall heat capacity of the reactant gas when the o-xylene concentration was changed. The inlet concentration was around 0.5 mole% and no more than a 30% step change in the concentration was carried out so that the maximum change in any physical property of the inlet gas would be less than 0.2%, which is negligible. It is conceivable that the thermocouple supposedly positioned at the centre line was in actual fact near the reactor wall; however if this anomalous behaviour occurred at the wall then surely it must also occur at the centre line of the reactor. The packing of the reactor was carried out in four steps with the packing density being within 1% of the final value for each of the sections, and even if there was a packing irregu-



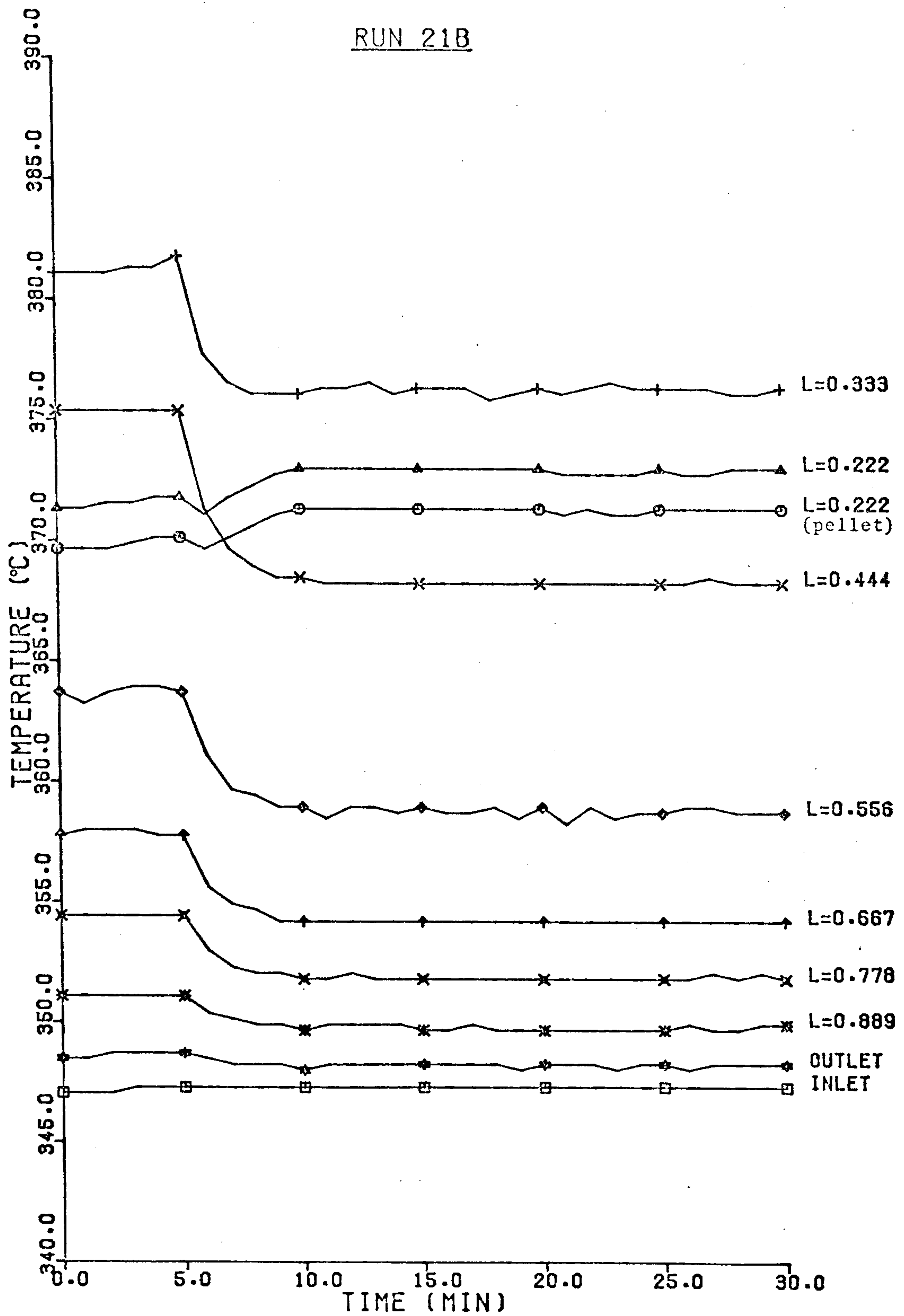
Graph 4.1. Experimental axial temperature profiles for an inlet xylene concentration step increase.



Graph 4.2. Experimental axial temperature profiles for an inlet xylene concentration step decrease.



Graph 4.3. Experimental transient for an inlet xylene concentration step increase.



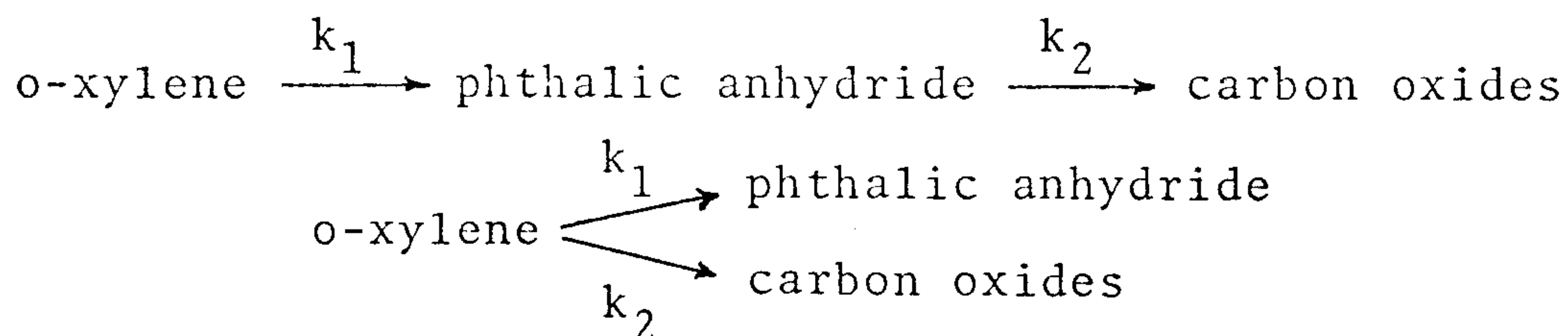
Graph 4.4. Experimental transient for an inlet xylene concentration step decrease.

arity which is very doubtful, it cannot give the results observed.

What initially appears to be wrong way behaviour at a point, can occur when the hot spot passes through the point; however in the experimental work carried out, the hot spot was always downstream from the dimensionless position 0.222, so this explanation is not possible. Initial wrong way behaviour has been demonstrated for a normal first order reaction in a catalytic reactor where the inlet temperature has been changed, but this does not lead to a stable steady state in the wrong direction unless multiple steady states are possible. This means that the only possible explanation remaining for the wrong way behaviour is some kinetic effect.

4.3i Reaction Model Discrimination

The variation in selectivity of the major products, where the phthalic anhydride/carbon oxides ratio decreases with increasing concentration and hot spot temperature can be explained by appropriate selection of the activation energies for any of the reaction networks surveyed in the literature review, chapter 2.1. The simplest possible models are the two following reaction schemes of two first order reactions in series or parallel



As the activation energy of the second reaction is slightly greater than that of the first, the yield of carbon oxides will increase as the temperature increases. It would not be necessary to allow for the small variation in the CO_2/CO ratio. These simple first order reaction models however, would not explain the wrong way behaviour of the first part of the axial temperature profile for an inlet o-xylene concentration increase as the heat evolved per unit length would increase over the first part of the reactor. To obtain wrong way behaviour the heat evolved must decrease over the first part of the reactor. This effect can only be achieved if the rate of one or both of the reactions concerned decreases; this in turn is dependent on at least one of the reactions having a negative apparent order of reaction over part of the concentration range.

All of the complex reaction schemes in the literature survey would be feasible, but only if a negative order of reaction could occur for some reactions. Using a model containing two reactions would mean the estimation of twice as many kinetic parameters, compared with the single reaction case from data where there is very little variation in the outlet concentrations. To simplify the modelling therefore, it is best to assume a single overall reaction, which must have a negative order of reaction at high o-xylene concentrations, with the selectivity and consequently the heat of reaction depending to a small extent on experimental results.

Obviously the simple power law expression is not a contender. The models derived by Mars and van Krevelen (3), Shelstad (4) and Hughes and Adams (5) all show, for varying o-xylene concentrations, a similar variation in the order of reaction; however this can only decrease from 1 to zero and cannot ever become negative. As only one overall reaction is being considered a summation expression as derived by Juusola is not suitable.

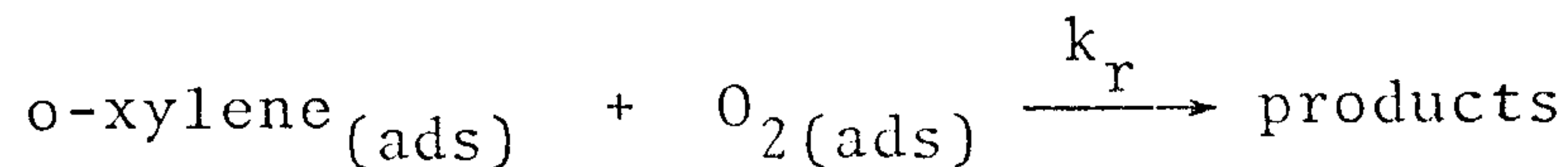
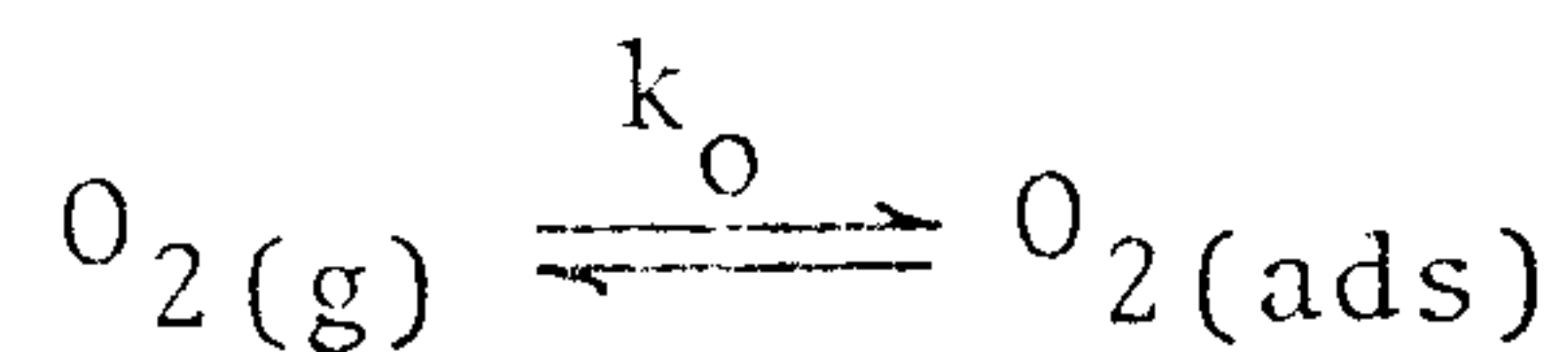
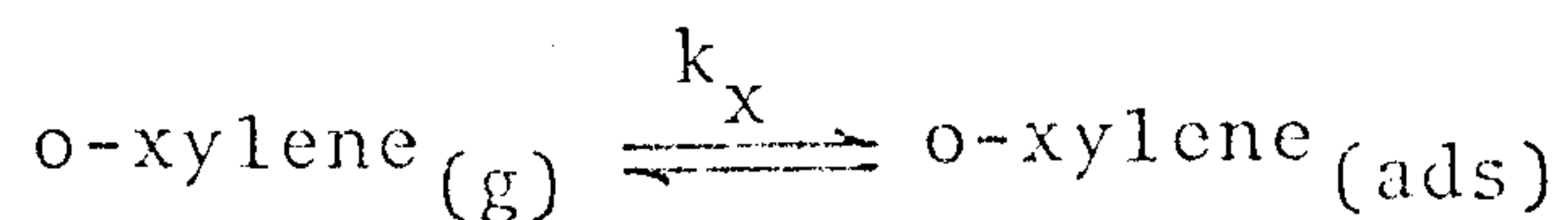
This leaves models that assume some form of catalyst deactivation (other than the redox type models previously mentioned), the bimolecular Langmuir-Hinshelwood model, and other models containing inhibiting effects due to the products formed. Obviously for the Langmuir-Hinshelwood model at high o-xylene concentrations, the order of reaction would become negative due to the squared denominator. For inhibiting models of the following forms:

$$R_r = \frac{k_r C_x}{1 + k_a C_{pa}}$$

$$R_r = \frac{k_r C_x^\alpha}{C_{pa}^\beta} \quad \text{where } \alpha > 0 \text{ and } \beta > 0$$

the variation in the apparent order of reaction with concentration is not obvious at first glance. By differentiating the rate of reaction according to $d(\ln R_r)/d(\ln C_x)$ (see appendix IX) the order of the reaction can be determined, and for neither of the forms above is a negative order of reaction possible.

The bimolecular Langmuir-Hinshelwood model is derived via the following steps:



where k_x and k_o are equilibrium adsorption constants.

The rate of reaction is proportional to the product of the adsorbed species.

$$R_r = k_r C_{\text{O}_2(ads)} C_{\text{x}(ads)}$$

which can be expressed as

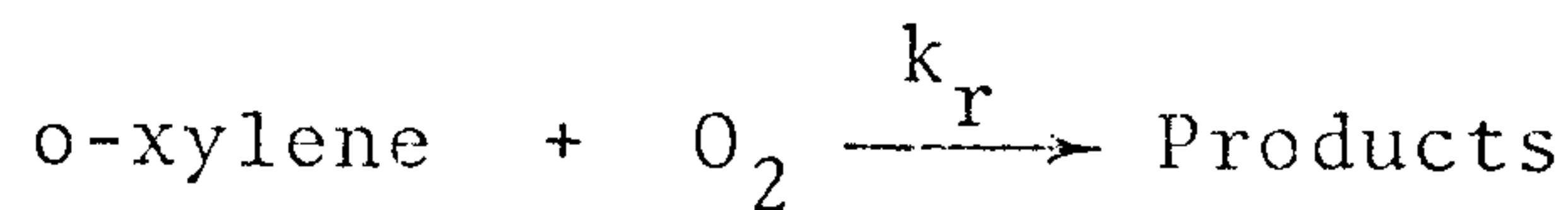
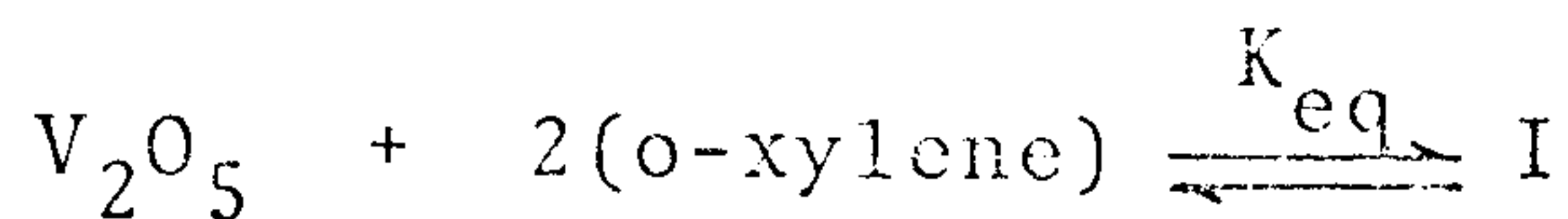
$$R_r = \frac{k_r k_o k_x C_{\text{O}_2} C_x}{(1 + k_o C_{\text{O}_2} + k_x C_x)^2}$$

For reaction at steady state where the oxygen concentration is approximately constant the full bimolecular Langmuir-Hinshelwood model can be simplified to:

$$R_r = \frac{k'_r C_x}{(1 + k_x C_x)^2}$$

When a dynamic situation occurs it may be necessary to consider the effect of the adsorption of oxygen by the catalyst, which would complicate the dynamic case appreciably. This would mean that two extra kinetic parameters would have to be evaluated in addition to those required at the steady state. Both parameters could have possible temperature variation.

The remaining option is some type of catalyst deactivation model. Consider the following equations:



The rate of reaction is proportional to the amount of V_2O_5 present.

$$R_r = k_r C_{V_2O_5} C_x$$

As the total number of active and inactive sites is assumed to be constant the overall rate of reaction can be expressed as:

$$R_r = \frac{k_r C_x}{1 + K_{eq} C_x^2}$$

The lower oxidation state of the catalyst I may be active, but in this study it is assumed to be inactive. As can be seen, the final form of the catalyst deactivation model is very similar to the simplified Langmuir-Hinshelwood model; (see appendix X for a normalised plot of these two models). At high o-xylene concentration both models can have an order of reaction that is negative. These two models are the simplest feasible set of reaction steps that could explain the wrong way behaviour, but are not necessarily the only alternative. Of the two models, the catalyst deactivation model is preferred as it has fewer kinetic parameters to be evaluated.

The next requirement of these two models is that for an increase in o-xylene concentration, the rate of reaction should initially increase, as observed experimentally

in the first part of the reactor before decreasing to a new steady state.

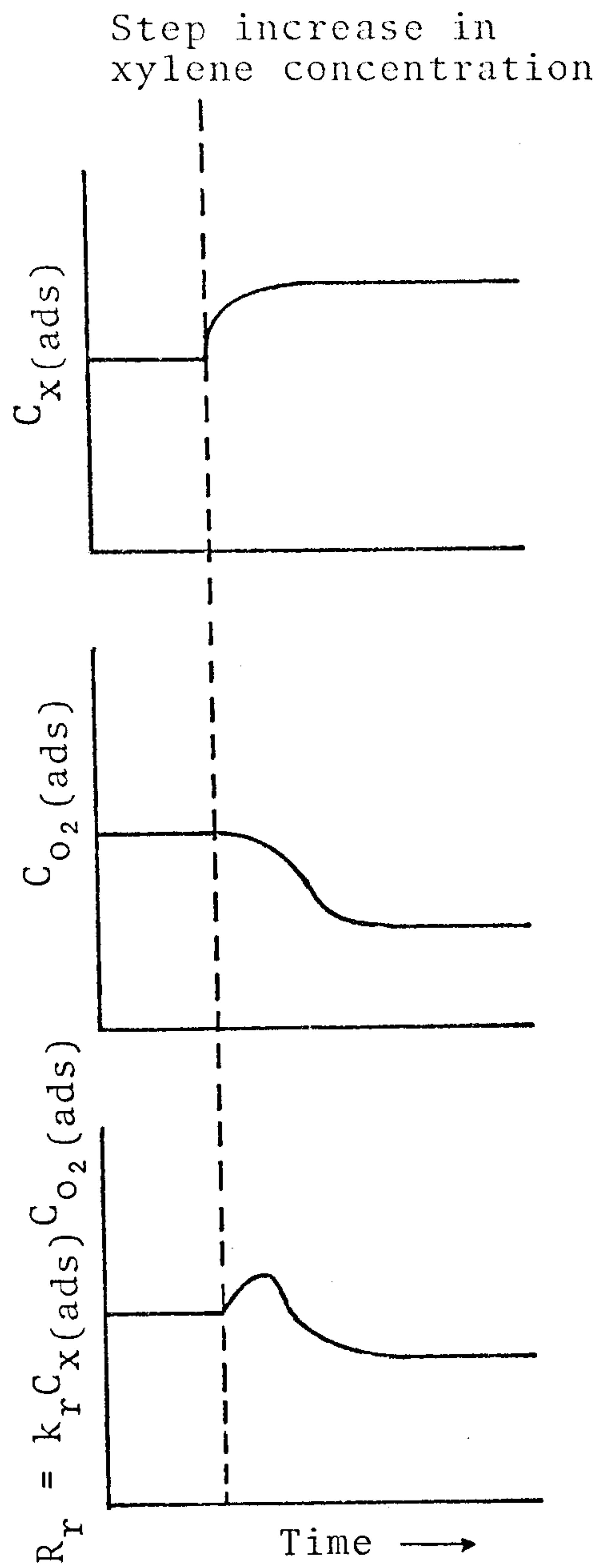
For the Langmuir-Hinshelwood model (see fig 4.1) an increase in the inlet o-xylene concentration results in an increase in the concentration of the o-xylene adsorbed on the catalyst. As a secondary effect the concentration of adsorbed oxygen must decrease due to the constant total number of active catalyst sites, but not necessarily by the same amount that the adsorbed o-xylene concentration has increased. The overall rate of reaction is the product of the concentration of the two adsorbed species resulting in the initial right way behaviour followed by the overall wrong way behaviour.

The response of the catalyst deactivation model to a step increase in the o-xylene concentration is simpler as the only transient effect is the decrease in the concentration of the catalytically active V_2O_5 sites. The product of o-xylene and the V_2O_5 sites is the overall rate of reaction. This shows a similar anomalous behaviour to that of the Langmuir-Hinshelwood model.

Other possible explanations of the initial right way behaviour are the effect of the heat of adsorption of the reactants on the catalyst, or the heat of reaction of the V_2O_5 to a lower oxidation state. Heats of adsorption are generally less in absolute terms than -2.0×10^5 KJ/Kmole, which is considerably less than the overall heat of

Langmuir-Hinshelwood

Model



Catalyst deactivation

Model

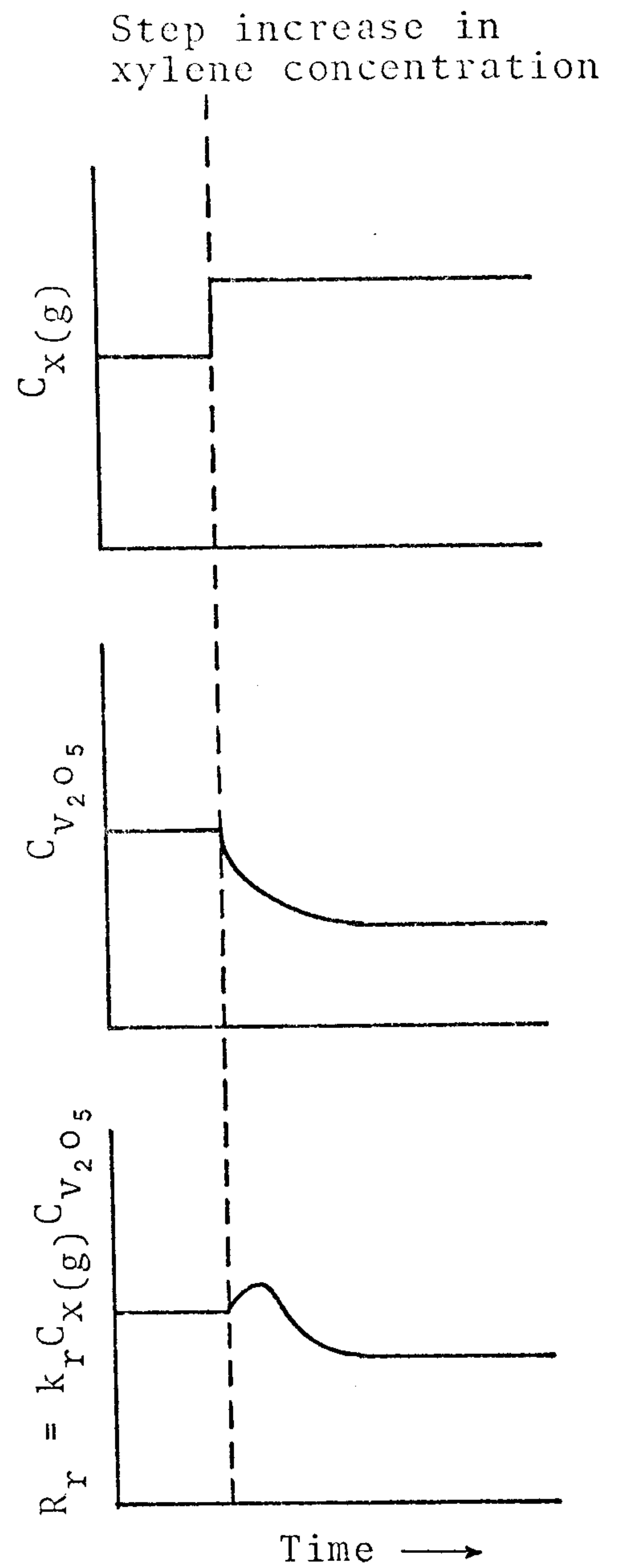


Fig 4.1. Two models that display the anomalous behaviour observed experimentally

reaction of -1.6×10^6 KJ/Kmole. This could not result in the observed initial right way behaviour of the axial temperature of up to 1.4°C . The reduction of V_2O_5 is endothermic so that this possibility is also eliminated.

As mentioned earlier the Langmuir-Hinshelwood model requires the evaluation of more kinetic parameters than the catalyst deactivation model so that the latter was preferred provided it could model the observed steady state behaviour satisfactorily.

For the case of only a single reaction the overall heat of reaction is obtained by summing the energy contributions for the formation of each product from o-xylene. The average contribution for each component was phthalic anhydride 52%, carbon dioxide 39%, carbon monoxide 7%, with the remaining 2% from the formation of maleic anhydride. Although no distinction could be made between o-tolualdehyde and maleic anhydride from the gas chromatographic analysis, the difference in assuming the former instead of the latter for the overall heat of reaction would be approximately 1% which is unimportant as this is within the analytical error .

4.4 Steady State Modelling

For an initial investigation of the reaction system the homogeneous partial differential equations were solved using both the Crank-Nicolson and the orthogonal collocation methods. For a simple case the Crank-Nicolson method

needed 30 radial solution points for comparable accuracy with the orthogonal collocation method using 6 radial points. If the solution of the temperature and concentration profiles is stored until the end of the calculation the orthogonal collocation method has the lower storage requirement. Conversely if the solution is printed out after every step the Crank-Nicolson method has a much lower minimum storage requirement. The computational time necessary for a "one off" calculation by either method is very similar. When the model has to be solved many times, as for a non-linear regression analysis, the collocation method is far superior. The Crank-Nicolson method is very wasteful as it has to completely restart for each regression iteration. Conversely, in the orthogonal collocation method for changes in some of the parameters (e.g. the kinetic parameters) the inverted solution matrices remain the same. These matrices need only be recalculated when other parameters (e.g. effective radial conductivity and wall heat transfer coefficients) are changed. For changes in the effective conductivity a large portion of the matrix, (see equations 3 and 9 of appendix III) for solution of the energy partial differential equation, has to be changed; while for a change in the wall heat transfer coefficient only some of the diagonal terms have to be changed. To speed up the calculation, a brief investigation was carried out to see if a small correction could be applied to the inverse to allow for small changes in the wall heat transfer coefficient. Although this was not rigorously investigated none of the simple schemes tried were of sufficient accuracy to make the operation successful.

For the matrices derived in the solution of the homogeneous equations as described in chapter 2.2, inversion by simple Gaussian elimination, with row pivoting, worked very successfully. The equations for the heterogeneous case, were ill-conditioned and it was necessary to use Crouts factorisation method to carry out the inversion.

In the homogeneous model six internal collocation points were used with less than 0.1°C variation from the case of five collocation points, up to a maximum hot spot temperature of 420°C . For the heterogeneous model, to save storage and computing time, only two internal collocation points were used up to a hot spot temperature of 400°C . Above this temperature, it was necessary to use four collocation points. The maximum error in all cases was less than 0.5°C .

4.4i Non-linear Regression Analysis

A selection of steady state axial temperature profiles, obtained from the initial and final steady states of the transient runs, were fitted by the method of non-linear regression of the kinetic and heat transfer parameters. The objective function was taken as the sum of squared errors between the experimental and the computed centre line temperatures at the same axial position. The sum of squares was minimised by the Powell conjugate direction method (100).

The inlet temperature was that measured experimentally with the sum of squares being calculated from 7 points between a dimensionless length of 0.222 and 0.889 inclusive. The last thermocouple at the outlet was not used as the temperature occasionally tailed off. This end effect was due to the surface of the lead/tin bath being level with this point resulting in a small amount of heat conduction up the tube. The point 0.111 was not included in the sum of squares due to the thermocouple failing as the result of the packing process.

The squared error between the theoretical and experimental concentration at the outlet of the reactor was not included in the modelling due to the arbitrary nature of selecting the necessary weighting factor and the need for an accurate fit for the temperature profiles for the transient modelling. As all the temperatures in the reactor bed were of the same order of magnitude, and were all measured in the same way, no weighting was applied to the individual temperatures. Although statistically correct, a natural consequence of this approach is that the hot spot temperature where most of the reaction takes place is given less weight than is perhaps desirable.

Preliminary trials modelling the axial reactor temperature profile of a single experiment as a first order reaction were reasonable; however this model could not be consistently applied to groups of data, and more complex models were investigated. Simultaneous non-linear regression analysis of all the data was not possible due to

limitations on computer time and storage. The minimisations were therefore carried out for groups of data having similar hot spot temperatures. Table 4.1 shows the results of the non-linear regression analysis for both the homogeneous and heterogeneous models using the catalyst deactivation rate of reaction.

$$R_r = \frac{k_o (\exp\{S - \frac{E_a}{R T}\}) C_x}{1 + K_{eq} C_x^2}$$

where C_x is expressed as a mole fraction of the total molar concentration (air + hydrocarbons), k_o is the dimensional constant ($1 \text{ Kmole/m}^3 \cdot \text{s}$) and S is the exponential frequency factor. By differentiating the rate equation it can be shown that a maximum rate of reaction occurs at a concentration of $1/\sqrt{K_{eq}}$. As the unusual effects previously mentioned occurred at least down to a concentration step between 0.39 and 0.31%, it was decided to fix this maximum rate of reaction at an intermediate value of 0.333%, therefore defining K_{eq} as 9.00×10^4 .

For the homogeneous model non-linear regression with four variables viz. frequency factor, activation energy, effective thermal conductivity and wall heat transfer coefficient proved to be unfeasible due to the high degree of correlation between the last two parameters. For runs 19 and 21, with moderate hot spot temperatures up to 395°C , the effective conductivity was fixed at $9.30 \times 10^{-4} \text{ KJ/m.s.}^\circ\text{C}$, which is just slightly above the majority of the correlations in chapter 2.4, thus greatly simplifying the search for the minimum sum of squares. The correlation between

Table 4.1 RESULTS OF NON-LINEAR REGRESSION ANALYSES

				Homogeneous Model			Heterogeneous Model		
Run No.	Inlet o-xylene Conc. (mole %)	Reynolds No.	Highest Recorded Temp. (°C)	Sum of Squares	Frequency Factor S	Stagnant Conductivity (k _e /k _g)	Sum of Squares	Frequency Factor S	Stagnant Conductivity (k _e /k _g)
19A _i	0.313	112.2	375.7	44.0	20.437	11.70	62.4	20.298	9.42
19B _i	0.397	111.4	381.8	22.4			26.0		
21A _f	0.392	112.1	382.3	24.7			34.7		
21B _f	0.324	112.7	376.4	21.3			34.4		
19B _f	0.515	111.4	390.6	59.9	20.386	11.70	44.3	20.283	11.91
21A _i	0.508	112.1	390.1	67.9			47.7		
22A _i	0.452	93.1	388.1	14.5			15.7		
22B _i	0.335	111.4	377.1	30.1			63.0		
23A _i	0.507	86.5	391.8	44.7	20.342	12.88	13.5	20.205	13.75
23A _f	0.444	94.3	383.0	15.5			29.6		
26A _f	0.545	112.9	402.2	144.4			141.9		
27B _f	0.529	112.9	399.4	106.7			109.0		
30A _i	0.524	111.4	402.2	59.4	20.400	19.6	53.5	20.255	18.9
30A _f	0.477	111.4	397.9	10.9			15.1		

In all cases the activation energy E_a is 1.105 x 10⁸ KJ/Kmole, and the wall heat transfer coefficient is defined by

$$Nu = 8.23 + 0.053 Re Pr$$

where i is initial steady state
f is final steady state.

the frequency factor and the activation energy was alleviated by the following standard transformation:

$$\begin{aligned} k_r &= \exp\left(S - \frac{E_a}{R T}\right) \\ &= \exp\left(S' - \frac{E_a}{R} \left\{ \frac{1}{T} - \frac{1}{T^*} \right\}\right) \end{aligned}$$

where $T^* = 623.^\circ\text{C}$

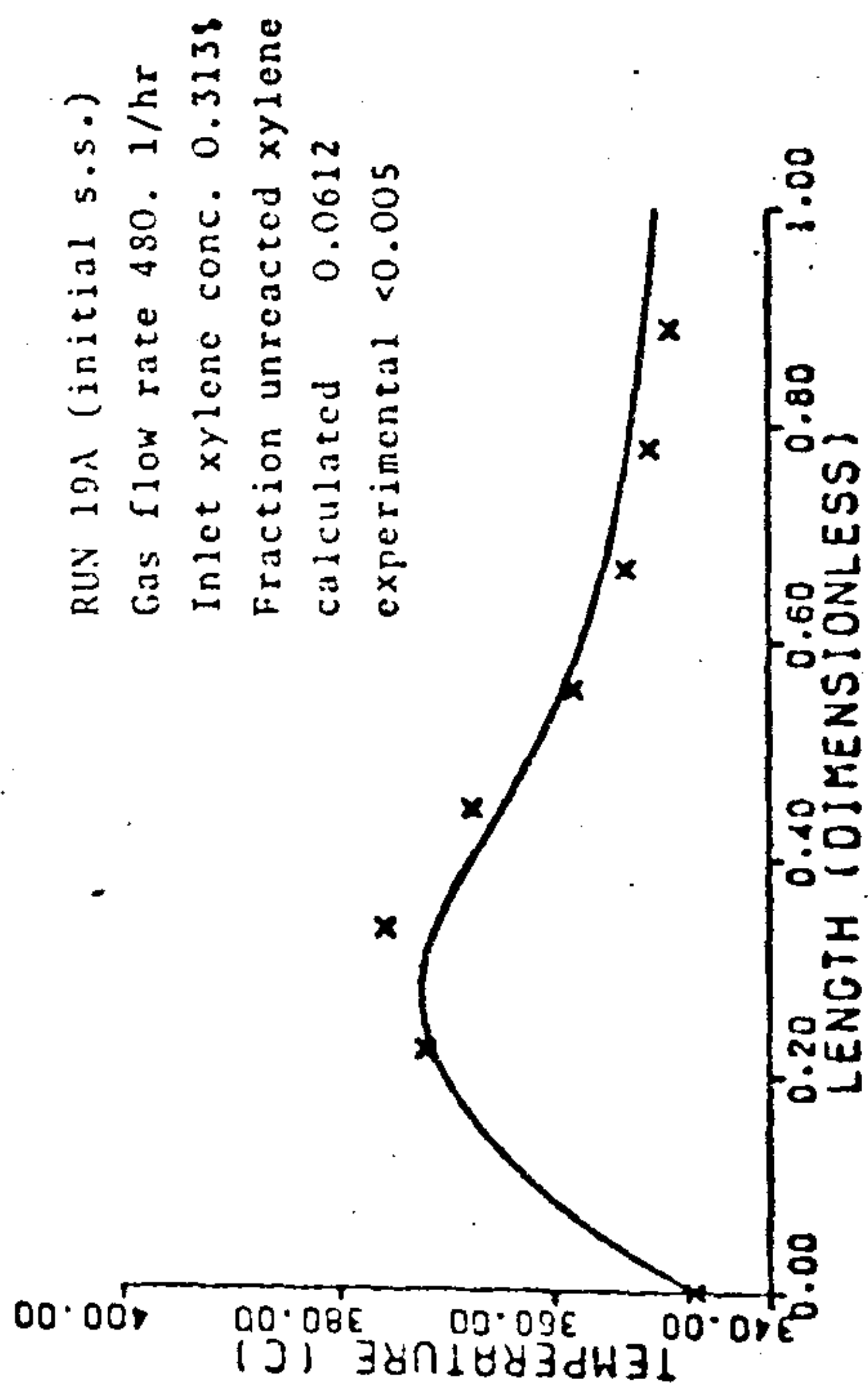
and $S' = S - \frac{E_a}{R T^*}$

The kinetic parameters directly determined from the regression analysis were the activation energy and the modified frequency factor S' .

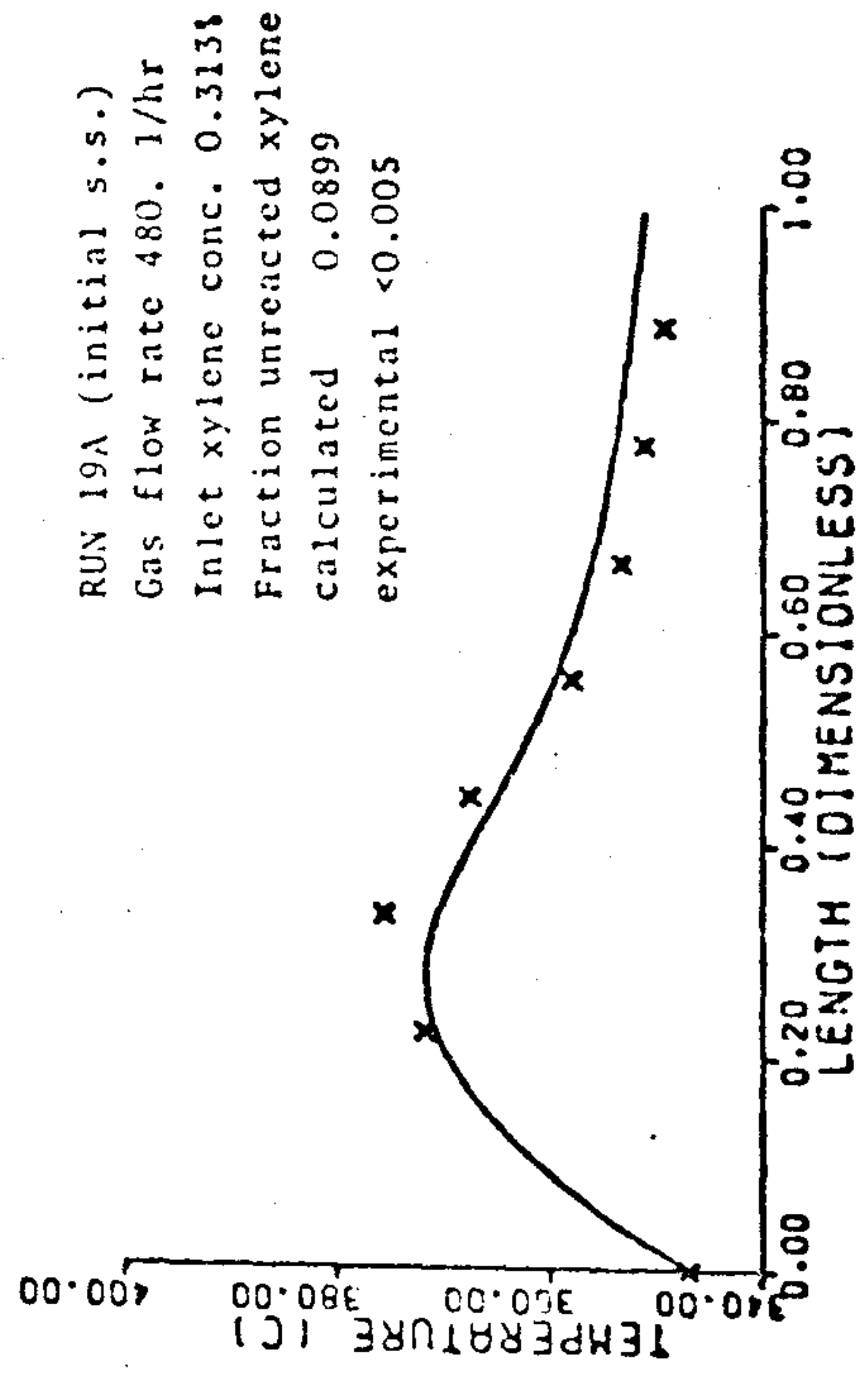
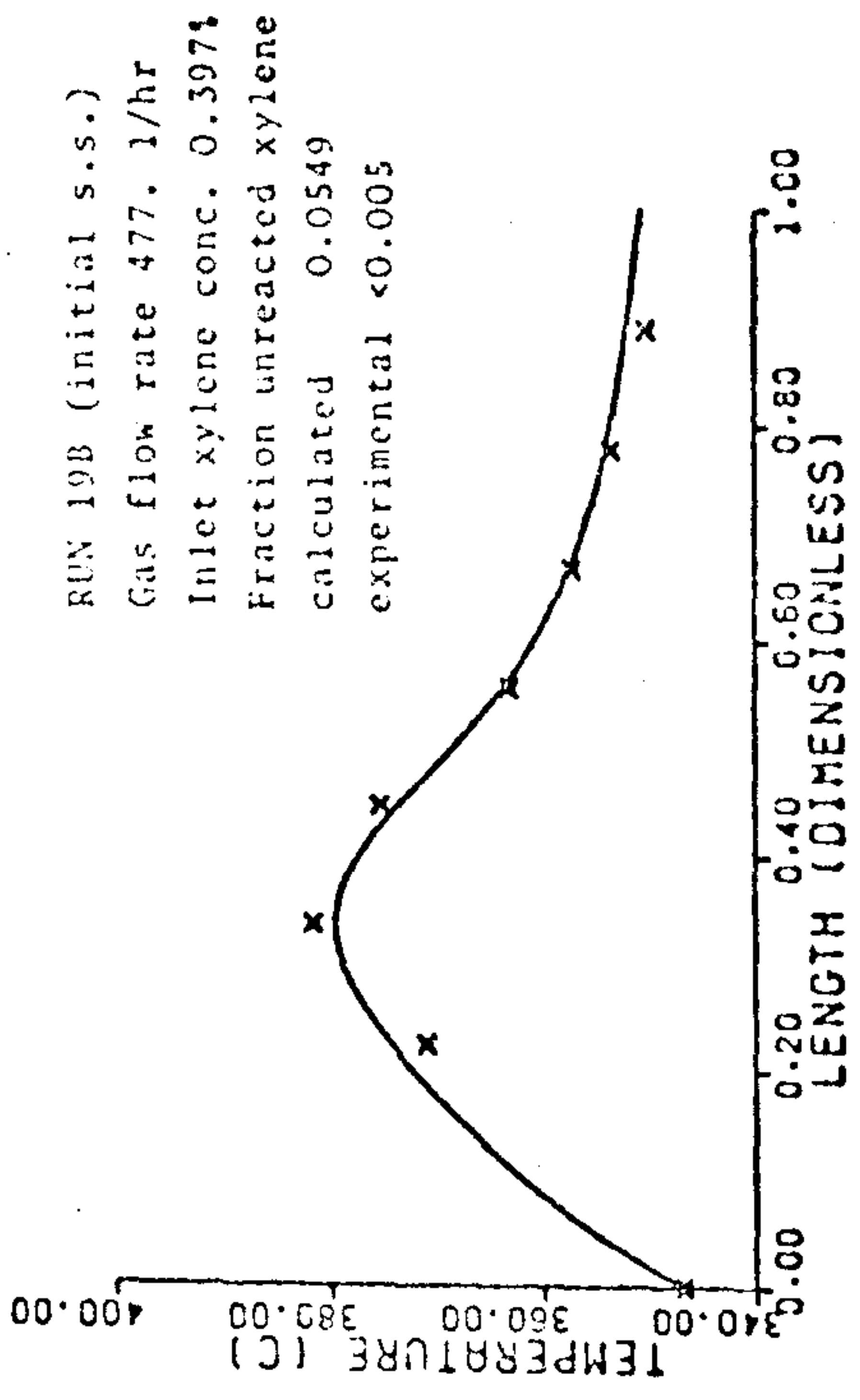
The resulting wall heat transfer coefficient for runs 19 and 21 was found to be $0.143 \text{ KJ/m}^2\text{s.}^\circ\text{C.}$, which is slightly greater than that derived from the correlations quoted in chapter 2.4, while the activation energy converged to $1.105 \times 10^8 \text{ KJ/mole}$. This is in the middle of the range of values found by most workers where mass transfer effects are not limiting. Most of the transient modelling was expected to be carried out based on the medium temperature experiments including runs 19 and 21, where no high temperature limiting effects occur. To simplify further regression analyses therefore, the activation energy was kept constant at this value for all the runs while the frequency factor was free to vary to account for any permanent catalyst deactivation as the experiments progressed.

As can be seen from table 4.1 and graphs 4.5 to 4.8 the overall fit obtained was good with the accuracy of the homogeneous model being equal to that of the more complex

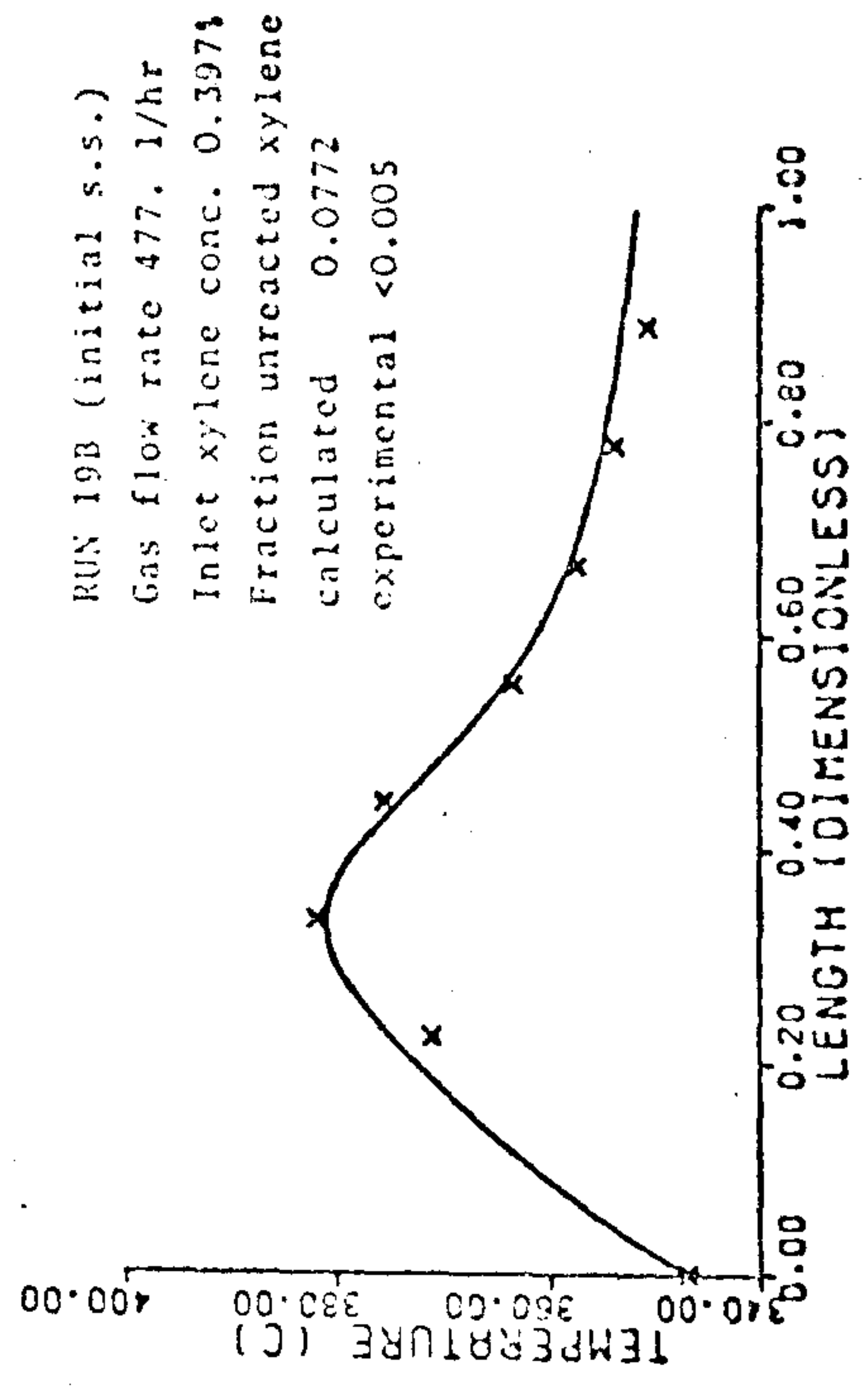
Graph 4.5 STEADY STATE MODELLING



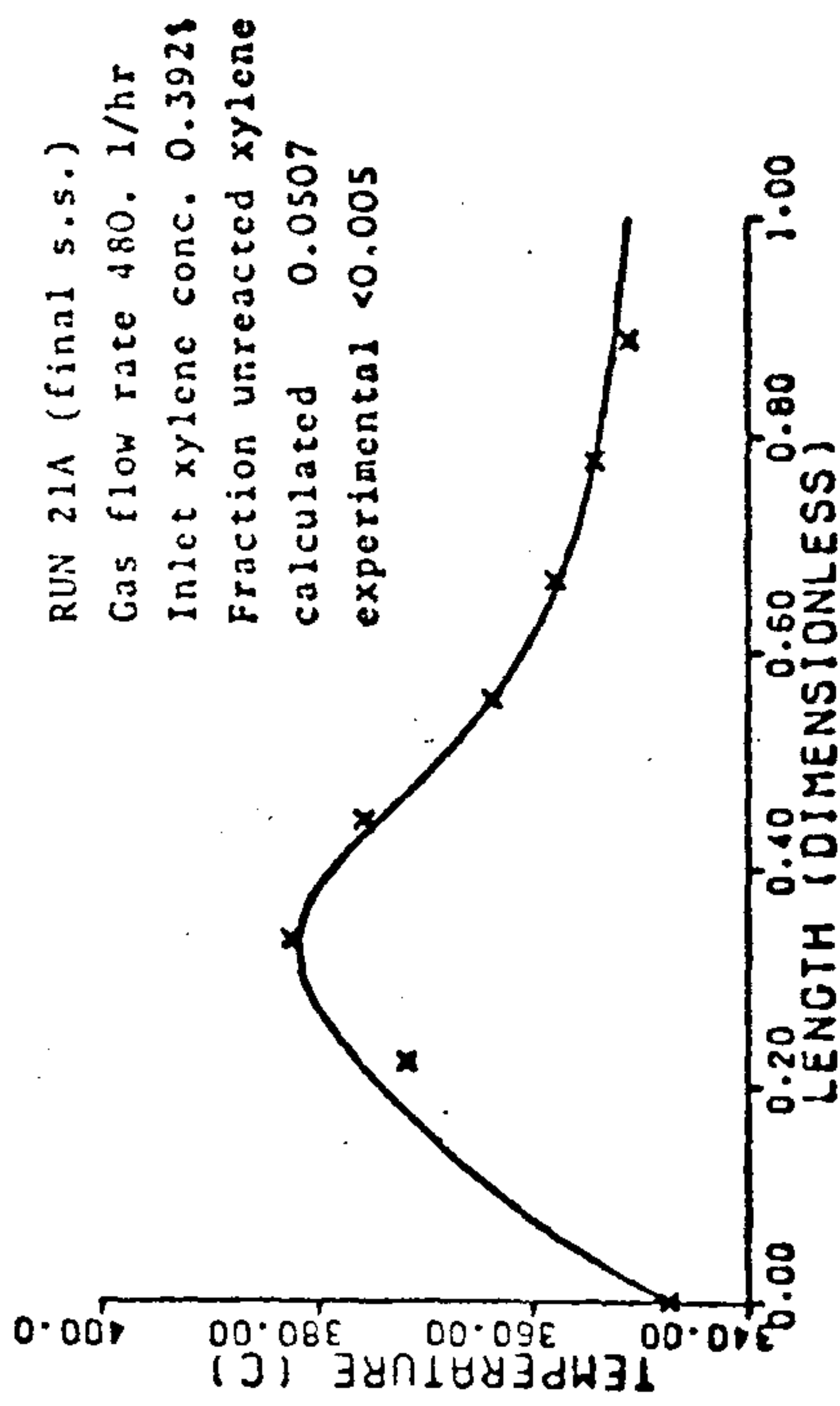
Homogeneous Model



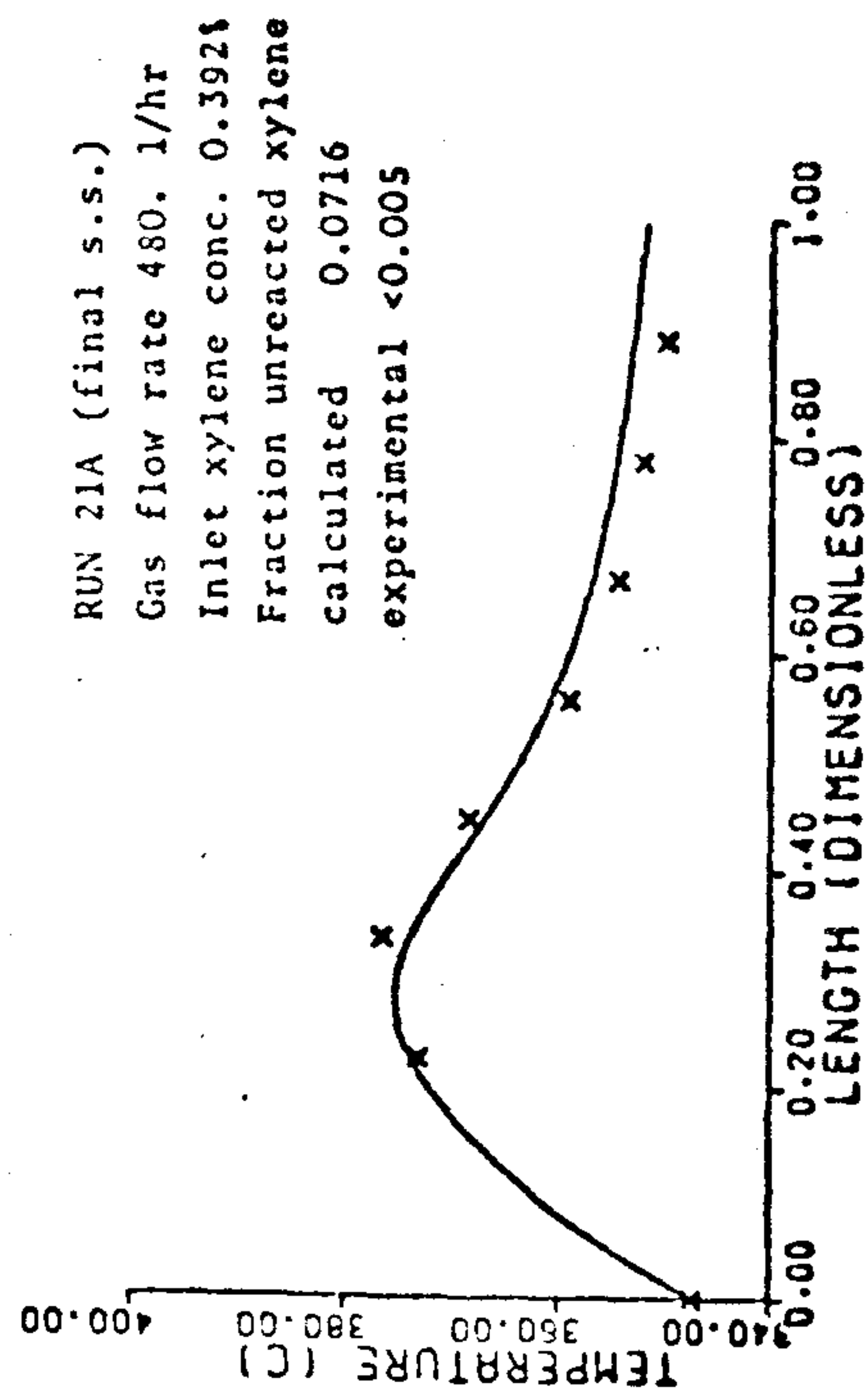
Heterogeneous Model



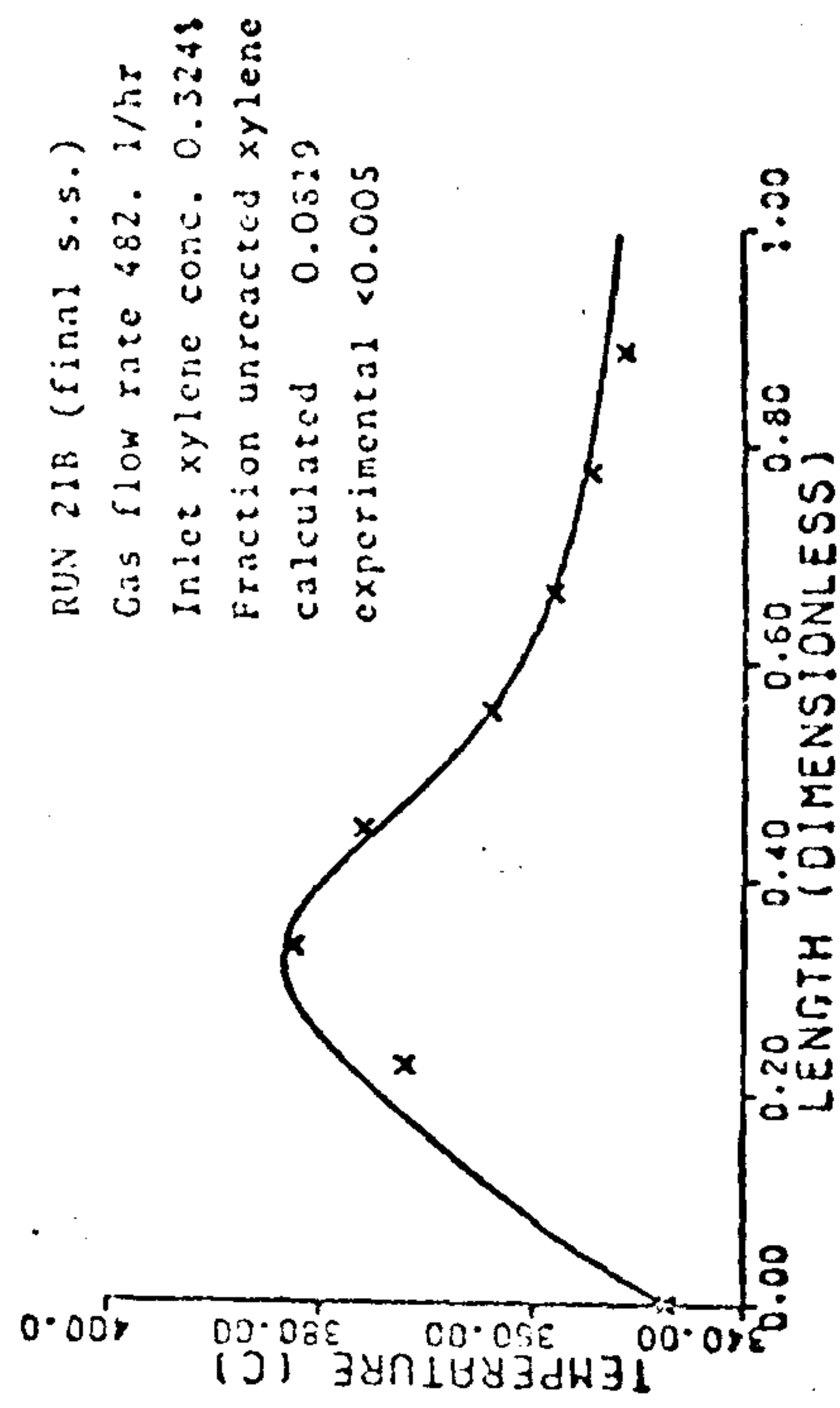
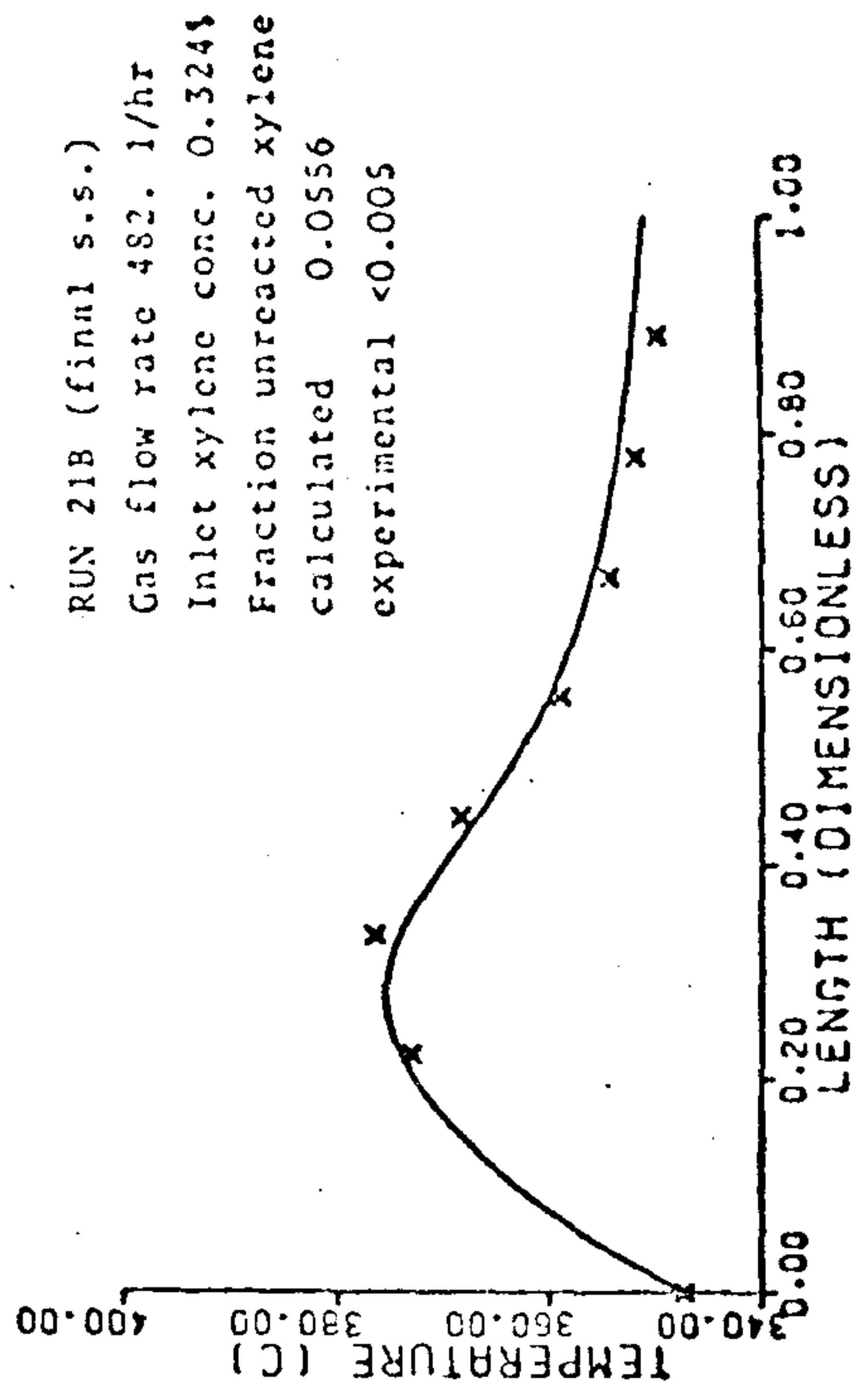
Graph 4.6 STEADY STATE MODELLING



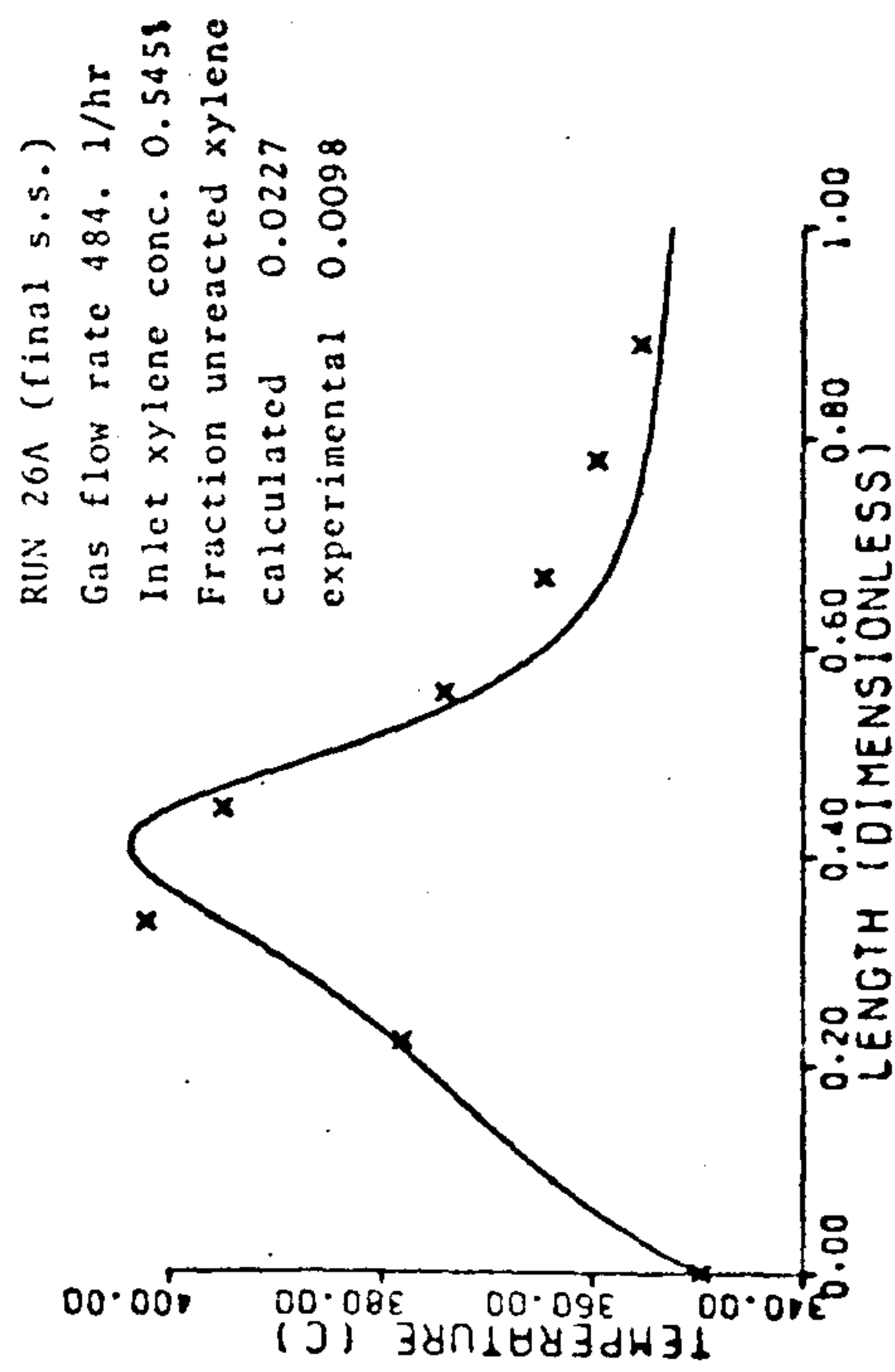
Homogeneous Model



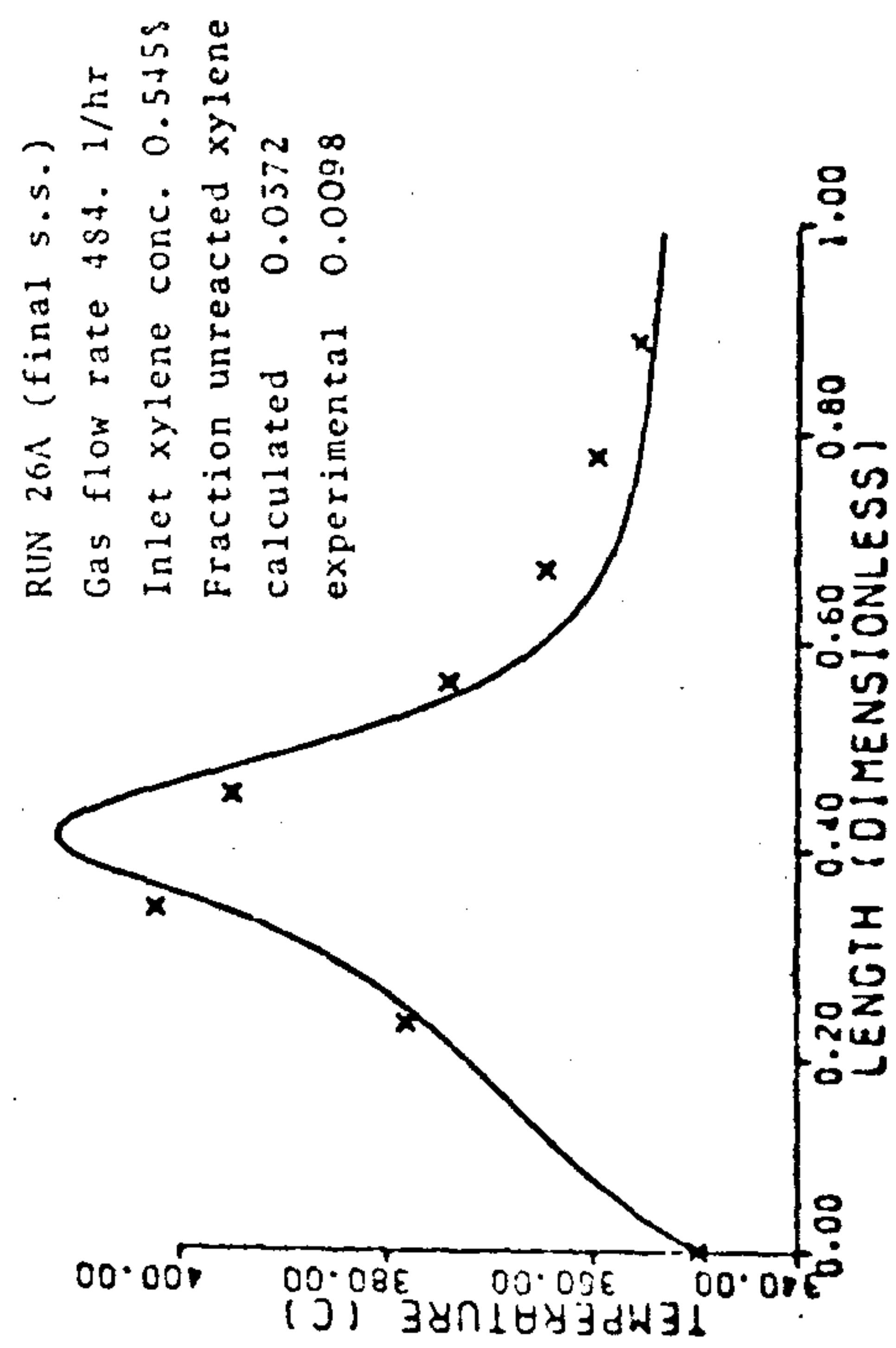
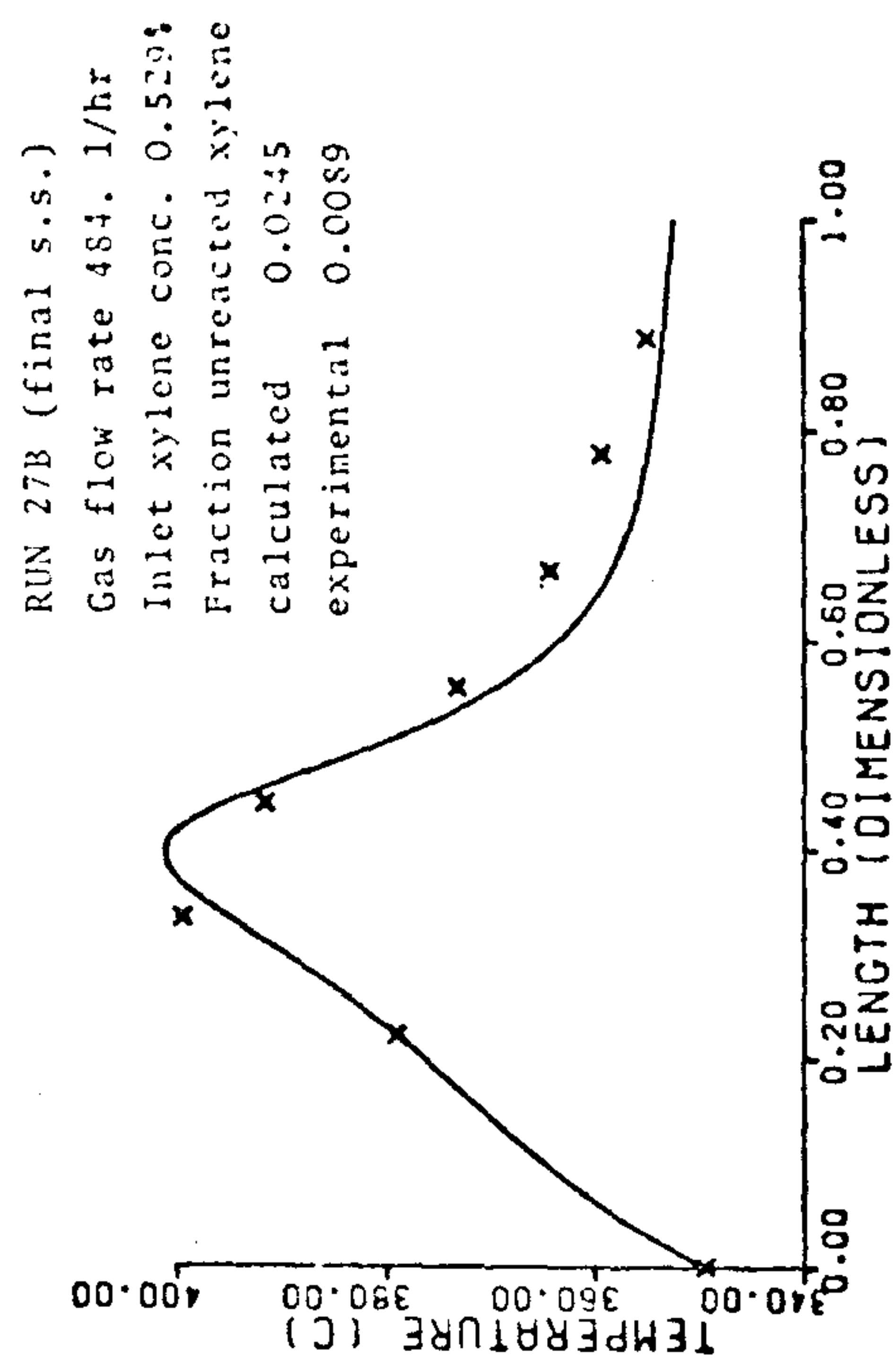
Heterogeneous Model



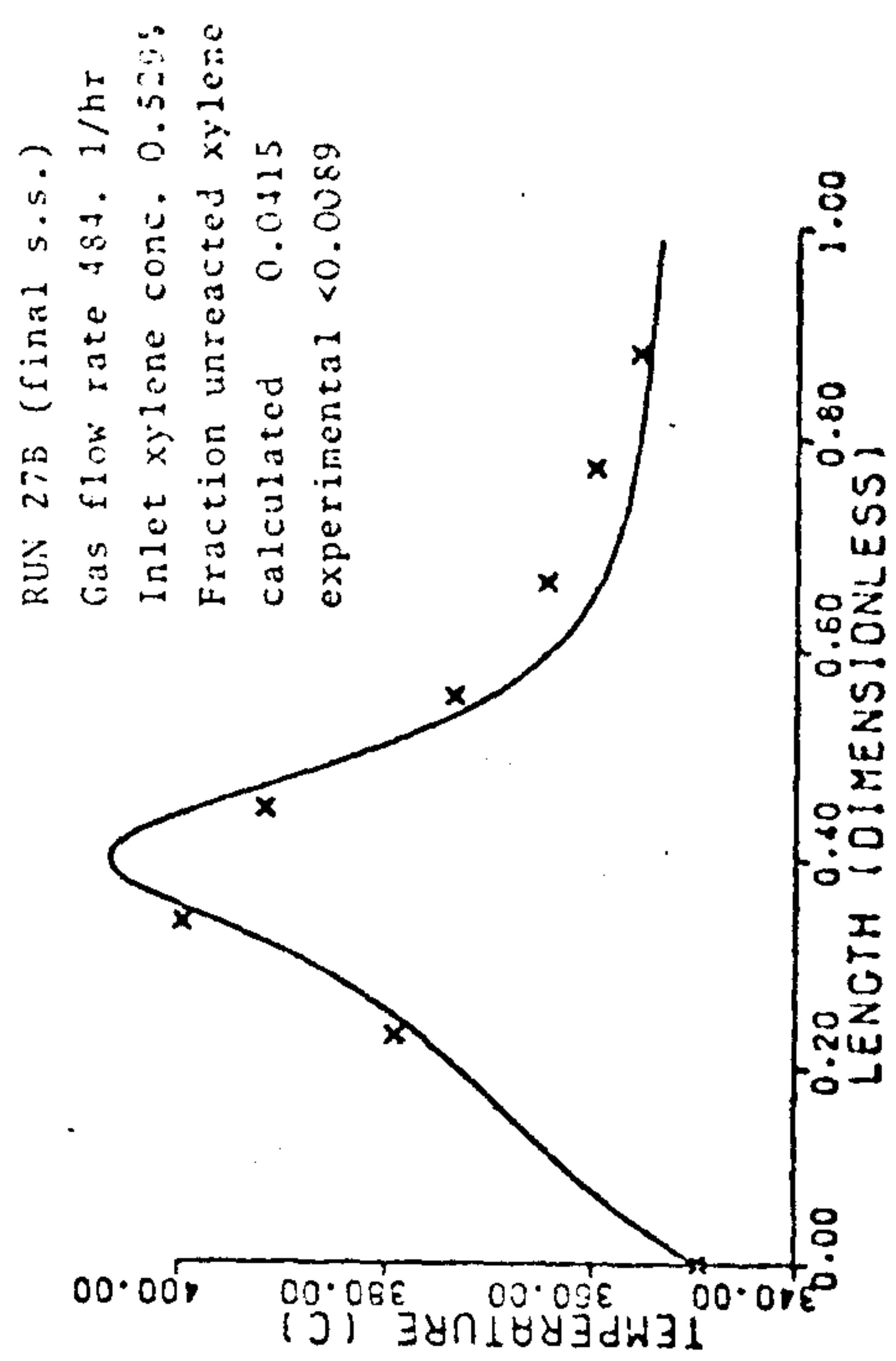
Graph 4.7 STEADY STATE MODELLING



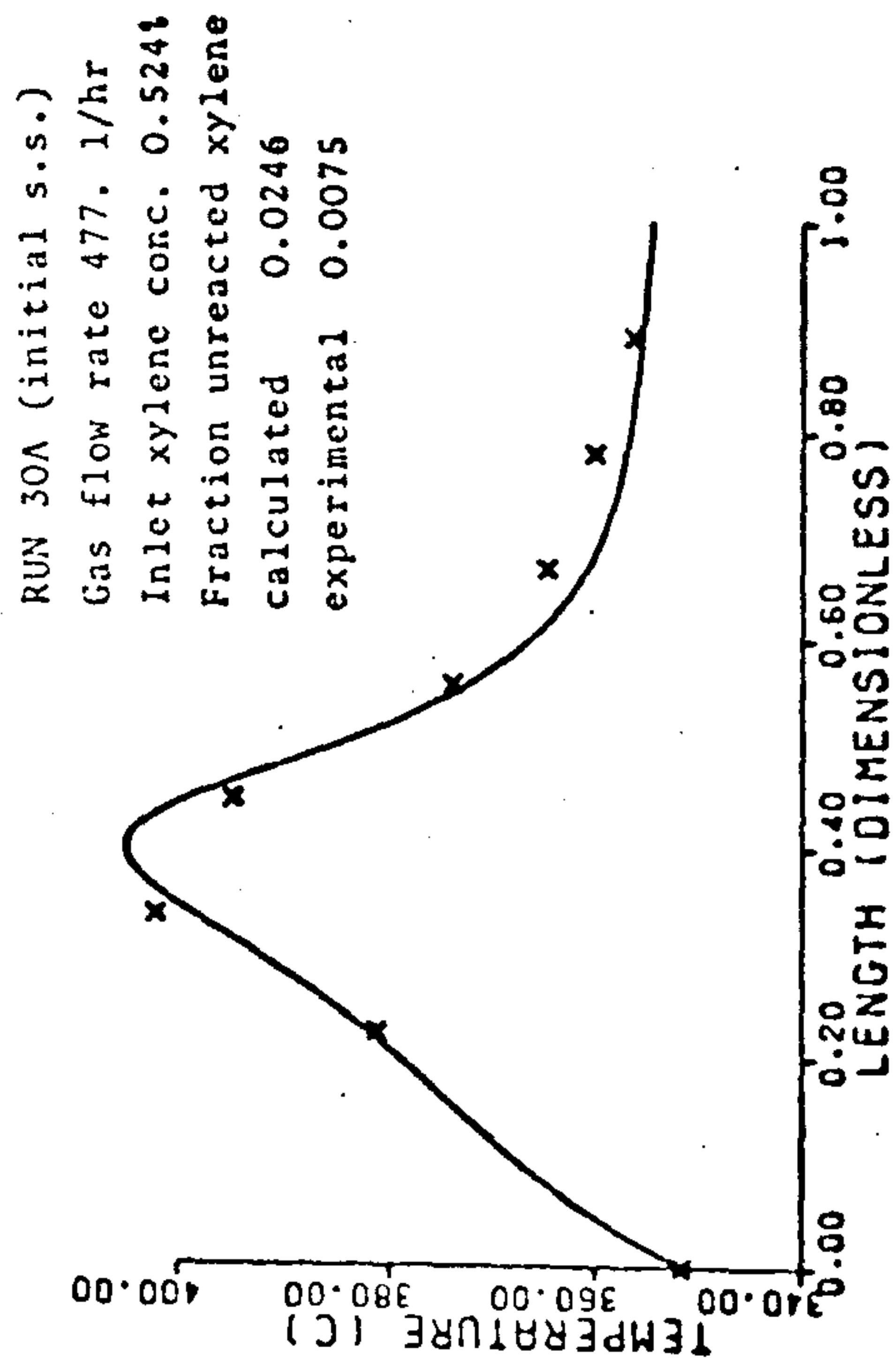
Homogeneous Model



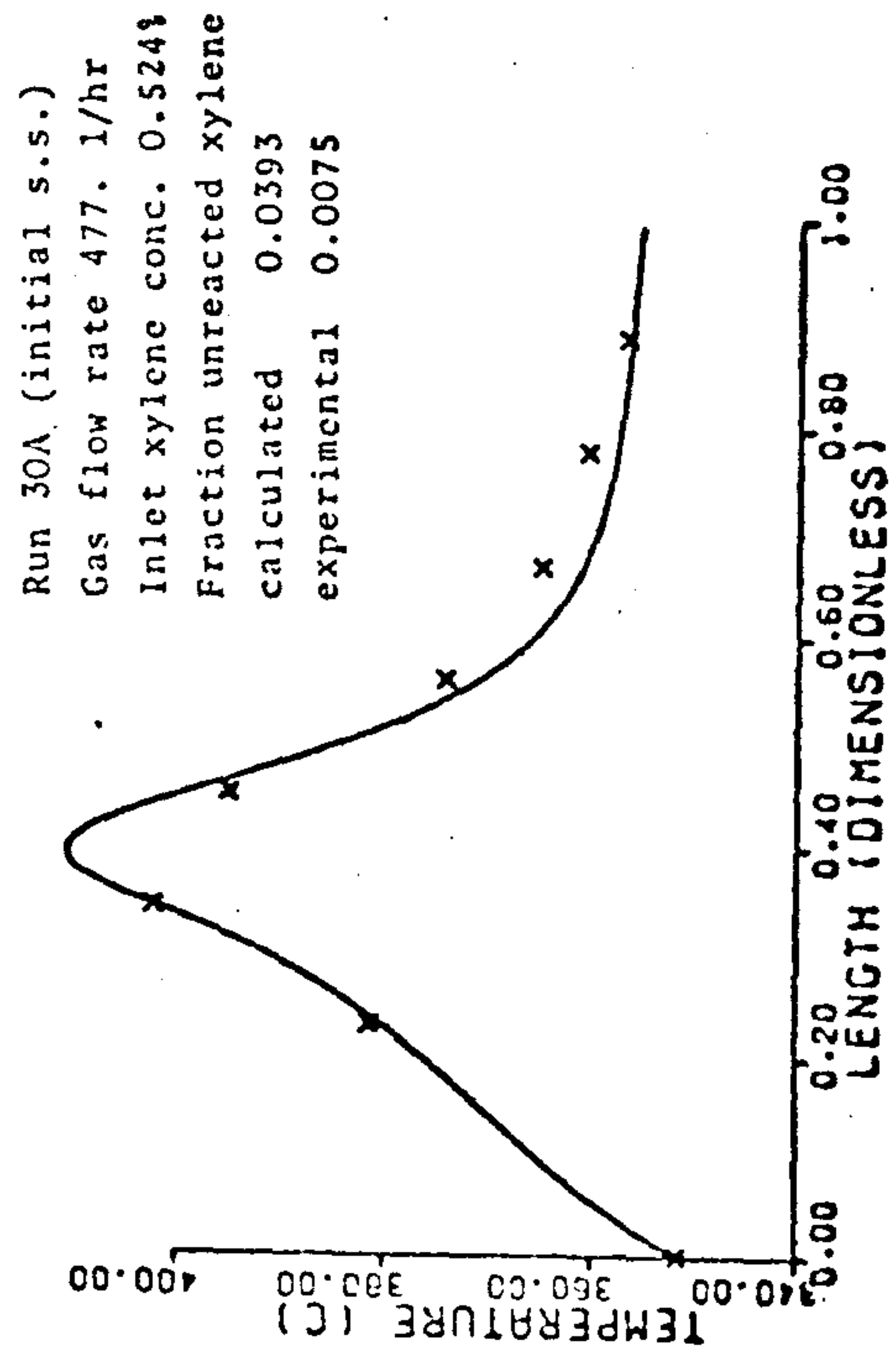
Heterogeneous Model



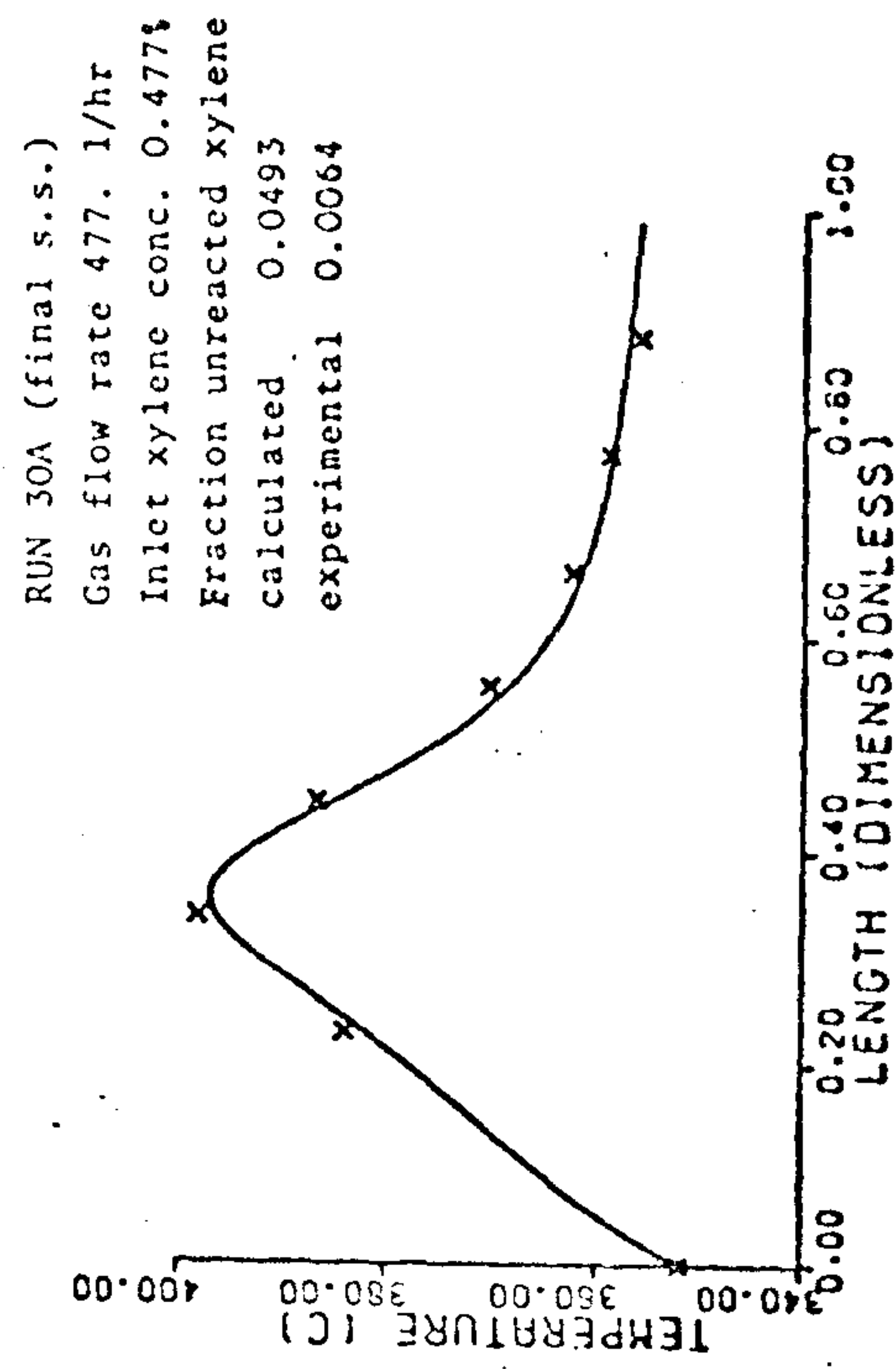
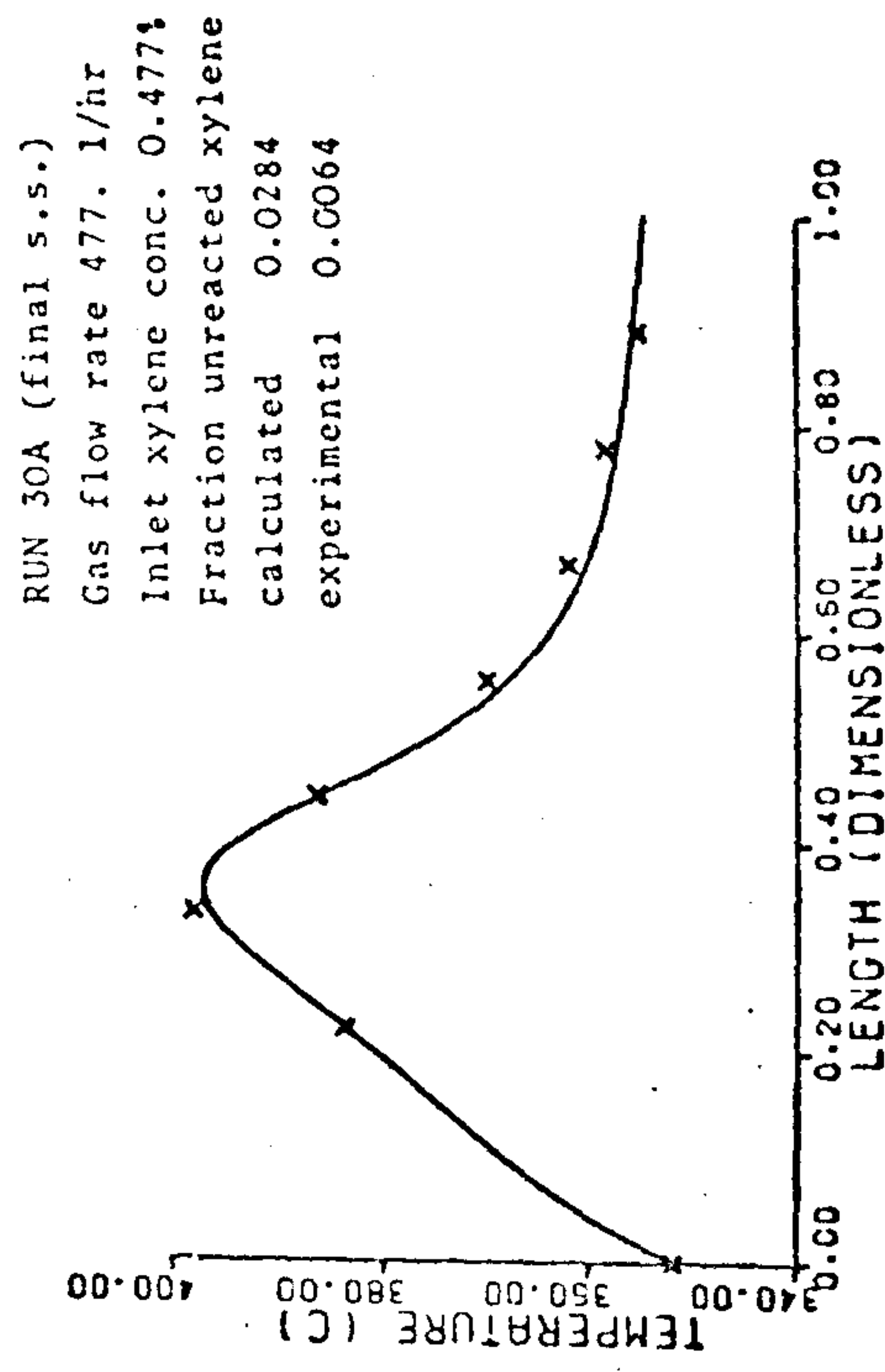
Graph 4.8 STEADY STATE MODELLING



Homogeneous Model



Heterogeneous Model



heterogeneous model.

Regression analysis based on the simplified bimolecular Langmuir-Hinshelwood model proved to be of the same degree of accuracy as that using the simpler catalyst deactivation model. Accordingly, no further modelling was carried out based on the Langmuir-Hinshelwood model due to the extra complexities in the transient case.

4.4ii Estimation and Effect of Heat and Mass Transfer

Parameters

The effect of the Peclet number for radial mass transfer was briefly investigated over a moderate range. As widely published, it was found that both the radial and axial temperature profiles were very insensitive to changes in this parameter.

The correlation between the effective thermal conductivity and the wall heat transfer coefficient for runs 19 and 21 is shown in table 4.2 and graph 4.9. This could be modelled within 1% error by an expression summing the resistances of the heat transfer effects by:

$$\frac{1}{U} = \frac{1}{h_w} + \frac{R}{1.91 k_e}$$

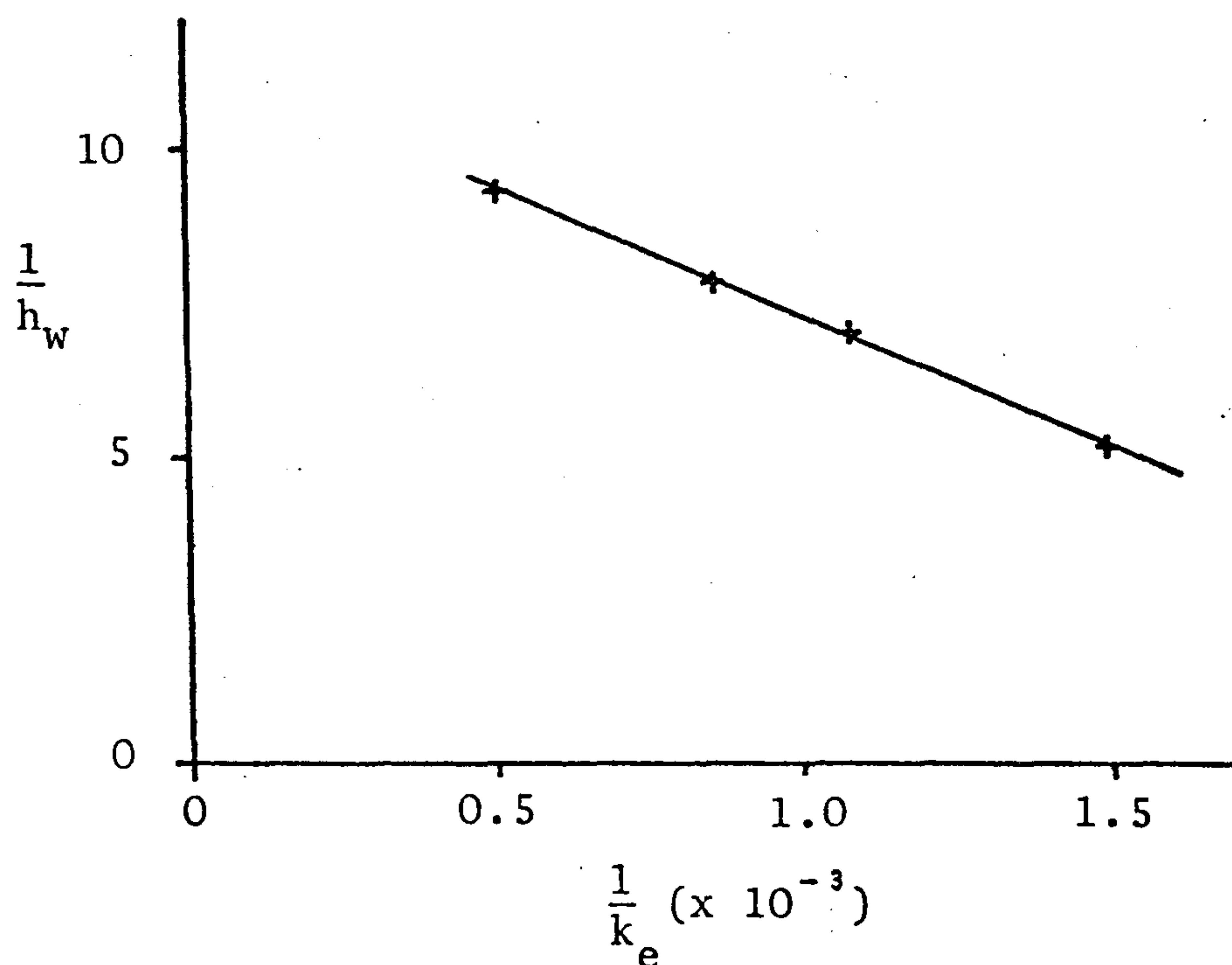
where $U=0.0882 \text{ KJ/m}^2 \cdot \text{s} \cdot ^\circ\text{C}$ and is a constant.

This form is identical to the overall one-dimensional heat transfer coefficient derived by Beek and Singer (101).

$$\frac{1}{U} = \frac{1}{h_w} + \frac{R}{4 k_e}$$

Table 4.2 RESULTS OF NON-LINEAR REGRESSION OF A
HOMOGENEOUS MODEL FOR RUN 19 AND 21 DATA

Effective Radial Conductivity $k_e \left(\frac{\text{KJ}}{\text{m.s.}^\circ\text{C}} \right)$	Wall Heat Transfer Coefficient $h_w \left(\frac{\text{KJ}}{\text{m}^2 \cdot \text{s.}^\circ\text{C}} \right)$	Activation Energy $E_a \left(\frac{\text{KJ}}{\text{Kmole}} \right)$	Exponential Frequency Factor S	Sum of Squares
6.74×10^{-4}	0.190	1.156×10^8	21.431	193.7
9.30×10^{-4}	0.143	1.105×10^8	20.437	172.2
11.6×10^{-4}	0.127	1.083×10^8	20.008	163.6
19.8×10^{-4}	0.108	1.020×10^8	18.806	151.9



Graph 4.9 CORRELATION OF HEAT TRANSFER PARAMETERS
FOR RUNS 19 AND 21

Crider and Foss (102)

$$\frac{1}{U} = \frac{1}{h_w} + \frac{R}{6.133 k_e}$$

and also the lumped one-dimensional heat transfer coefficients derived in appendix II by application of the orthogonal collocation method to the case of one internal collocation point. The only difference is the value of the constant in the denominator of the conductivity term, which was found to be significantly lower in this study. The correlations of Crider and Foss, and Beek and Singer were theoretically derived under non-reactive conditions. The experimental difference may be due to the reaction itself and/or the appreciable variation in the activation energy necessary to obtain the converged sum of squares on varying the heat transfer parameters. The high value of the diameter ratio used may also affect the constant.

To eliminate the correlation of the heat transfer parameters therefore it may be possible to carry out a transformation similar to that for the kinetic parameters. If U and either h_w or k_e are used as the parameters for non-linear regression the problem may be overcome.

To model the wall heat transfer coefficient and the effective radial conductivity for various flow rates, correlations of the following form were used.

$$\begin{aligned} Nu &= Nu^0 + \lambda Re Pr \\ \frac{k_e}{k_g} &= \frac{k_e^0}{k_g} + \phi Re Pr \end{aligned}$$

where $\lambda=0.054$ as suggested in chapter 2.5. The wall heat

transfer coefficient for runs 19 and 21 of $0.143 \text{ KJ/m}^2 \cdot \text{s} \cdot ^\circ\text{C}$ at a Reynolds number of 112, completely defines the wall heat transfer correlation as

$$\text{Nu} = 8.23 + 0.054 \text{ Re Pr}$$

This is the same as the correlation originally selected in chapter 2.5. The effective radial conductivity value of $9.30 \times 10^{-4} \text{ KJ/m} \cdot \text{s} \cdot ^\circ\text{C}$ was just slightly greater than the correlations surveyed in chapter 2.4. If $\phi=0.053$, as suggested in chapter 2.4, then at a Reynolds number of 112 the stagnant conductivity term is 15.3. Increasing ϕ to 0.10 reduces the stagnant conductivity to a more realistic 11.7, which is not too different from the suggested value of 10. Yagi and Kunii (62) in their work on annular packed beds show that for the diameter ratio (D_p/D_t) of 0.268 used in this study, the stagnant Nusselt number increases to 18, however there is no other work to support this result. If this were the case then by extrapolating the correlation derived for the overall heat transfer coefficient U , at a Reynolds number of 112, the effective radial conductivity must be $5.51 \times 10^{-4} \text{ KJ/m} \cdot \text{s} \cdot ^\circ\text{C}$ which would give the choice of either of the following equations

$$\frac{k_e}{k_g} = 7.39 + 0.053 \text{ Re Pr}$$

$$\frac{k_e}{k_g} = 3.74 + 0.10 \text{ Re Pr}$$

The first correlation with the slope of 0.053 results in a stagnant conductivity of 7.39 which is less than the original correlation recommended but very close to the value of 8.0 calculated by the theoretical equation of

Kunii and Smith (60). The stagnant conductivity in the second correlation is now much lower than the range of experimental data presented in fig 3.1 and cannot be considered feasible. The correlations based on a stagnant Nusselt number and a stagnant effective conductivity ratio of 18 and 7.39, respectively could be used, and may result in a lower sum of squares than originally obtained, as shown by the trend in table 4.2. The supporting evidence for this is even more sparse than for the original correlations derived from runs 19 and 21. Unfortunately there is very little literature on heat transfer correlations at the high D_p/D_t ratios occurring in the catalytic oxidation of o-xylene. Although changing the heat transfer parameters (see table 4.2) causes a noticeable change in the kinetic parameters, the change in the axial temperature profile is minimal as long as the overall heat transfer correlation for U is obeyed.

To obtain a reasonable fit at high inlet o-xylene concentrations and consequently high hot spot temperatures it was necessary to increase the amount of heat removed from the system by either increasing the wall heat transfer coefficient or the effective radial conductivity. It was decided to hold the former constant as this should be more stable to temperature variations and vary the latter as this may include some effect of axial dispersion of heat. The wall heat transfer correlation used throughout the modelling was that originally derived from the non-linear regression of runs 19 and 21 with a stagnant Nusselt number of 8.23. As shown in table 4.1 the stagnant

conductivity had to be increased from 9.42 to 26.0 as the inlet o-xylene concentration increased. This corresponds to an increase in the effective conductivity from 9.30×10^{-4} to 16.2×10^{-4} KJ/m.s.°C for the homogeneous model. A similar increase was necessary for the heterogeneous model.

The necessity of increasing the effective radial conductivity as the hot spot temperature increases may be due to limiting of the reaction by film mass transfer effects, a decrease in the catalyst activity or the effect of axial dispersion becoming important. As can be seen from graphs 4.5 to 4.8 the experimental points show that an improved fit could be obtained if the axial temperature profile was slightly stretched, which would occur if axial dispersion were included. As the inclusion of axial dispersion appreciably complicates the solution of the equations, this has not been quantitatively studied.

For the non-linear regression analysis carried out using the heterogeneous model the sum of squares was determined from the difference between the calculated bulk gas temperature and the measured temperature, while the reaction rate was calculated for the temperature and concentration at the pellet. The pellet heat and mass transfer coefficients were not free to vary but were fixed from the literature correlations as suggested in chapter 2.6. Typical axial temperature profiles for the heterogeneous modelling are shown in graphs 4.5 to 4.8. As the heterogeneous model not only includes the radial effective conductivity, which is a parameter in the homogeneous model, but also the heat

transfer from the pellet to the gas, for an accurate fit it may be necessary to have a lower radial conductivity in the heterogeneous case compared to the homogeneous case. This was true at all temperatures. At higher temperatures the difference was much less as can be seen by comparing the stagnant conductivity term in table 4.1.

The effect of varying the mass transfer coefficient is shown in table 4.3. At low hot spot temperatures (runs 19 and 21), decreasing the pellet mass transfer coefficient increases the converged sum of squares though not necessarily by a significant amount. At high temperatures however, the sum of squares is significantly decreased, improving the fit. Increasing the pellet heat transfer coefficient has a similar effect but to a lesser degree. The lower mass transfer coefficient results in a lower value of the effective radial conductivity for the higher temperature runs. Slightly less overall variation is therefore necessary in the effective conductivity than that originally determined for both the homogeneous and heterogeneous models.

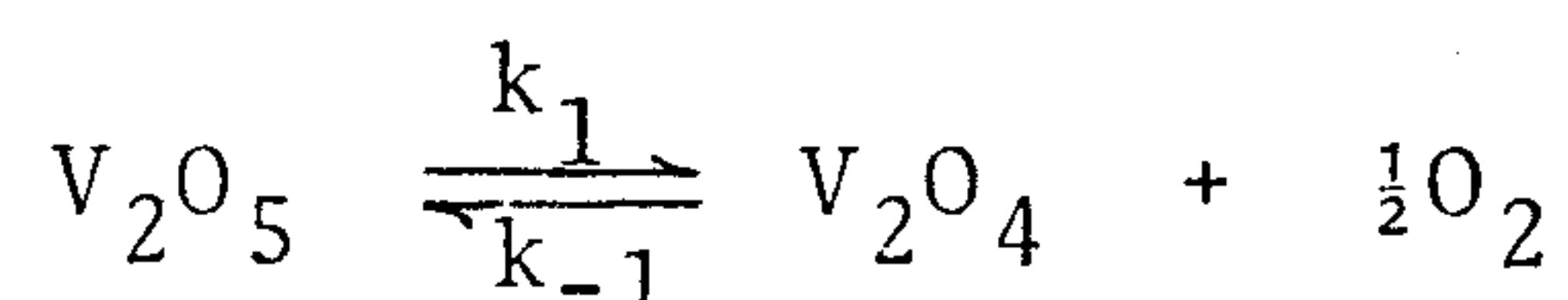
The improved fit at high temperatures by more than halving the pellet mass transfer coefficient ordinarily would imply that the original mass transfer coefficient obtained from the literature was in error by 100%, and that mass transfer is the controlling resistance at higher temperatures. If the mass transfer coefficient is halved then the heat transfer coefficient must also be halved to keep the ratio j_h/j_d equal to 1.08 (see the literature survey chapter 2.6). Regression analysis of runs 26 and 27 with

Table 4.3 RESULTS OF VARYING THE FILM MASS
TRANSFER COEFFICIENT

Run No.	$K_G = 0.163 \text{ m/s}$		$K_G = 0.0740 \text{ m/s}$	
	Effective Radial Conductivity $k_e \left(\frac{\text{KJ}}{\text{m.s.}^\circ\text{C}} \right)$	Sum of Squares	Effective Radial Conductivity $k_e \left(\frac{\text{KJ}}{\text{m.s.}^\circ\text{C}} \right)$	Sum of Squares
19	8.22×10^{-4}	88.4	7.44×10^{-4}	123.4
30	12.7×10^{-4}	66.0	10.0×10^{-4}	23.0
26/27	16.7×10^{-4}	246.4	11.8×10^{-4}	41.2

Note. $K_G = 0.163 \text{ m/s}$ was the original value derived from the correlations for the mass transfer coefficient at a Reynolds number of 112.

both coefficients halved resulted in the original sum of squares, obtained using the literature correlation for the transport coefficients. Therefore mass transfer cannot be the limiting effect at the maximum temperature of 410°C reached in the modelled experiments. Most workers on this system agree that mass transfer limitation occurs around 440°C. Other possible effects as mentioned previously are the increased importance of the axial dispersion of heat at high hot spot temperatures or a change in the oxidation state of the catalyst. For simplicity in the catalyst deactivation model no temperature dependence of the catalyst equilibrium constant has been included by introduction of an activation energy parameter. If more deactivated catalyst were present at higher temperature then this would explain the slowing of the reaction at higher temperatures and give the same result as decreasing the mass transfer coefficient to give mass transfer control. Vijn (103) states that for the reaction



the activation energies are 1.56×10^8 and 1.80×10^8 KJ/Kmole for the forward and reverse reactions respectively. This would favour more V_2O_5 at higher temperatures. The inactive species may therefore be $\text{V}_2\text{O}_{4.34}$ with the further formation of inactive V_2O_3 , at high temperatures, appreciably decreasing the reaction rate. The slowing of the reaction at high temperatures may also be influenced by axial heat dispersion as for a hot spot of 420°C the maximum axial temperature gradient is 400°C/m.

For run 32, where the hot spot temperature reached 440°C, no reasonable degree of fit was achieved by either the homogeneous or heterogeneous models. This may have been due to film mass transfer limitation at the higher temperature or to the large degree of temporary catalyst deactivation.

Over all the runs carried out there was no evidence of permanent deterioration in the activity of the catalyst. The exponential frequency factor S derived from all the modelling carried out, varied between 20.3 and 20.5 for the homogeneous model and 20.2 to 20.3 for the heterogeneous model.

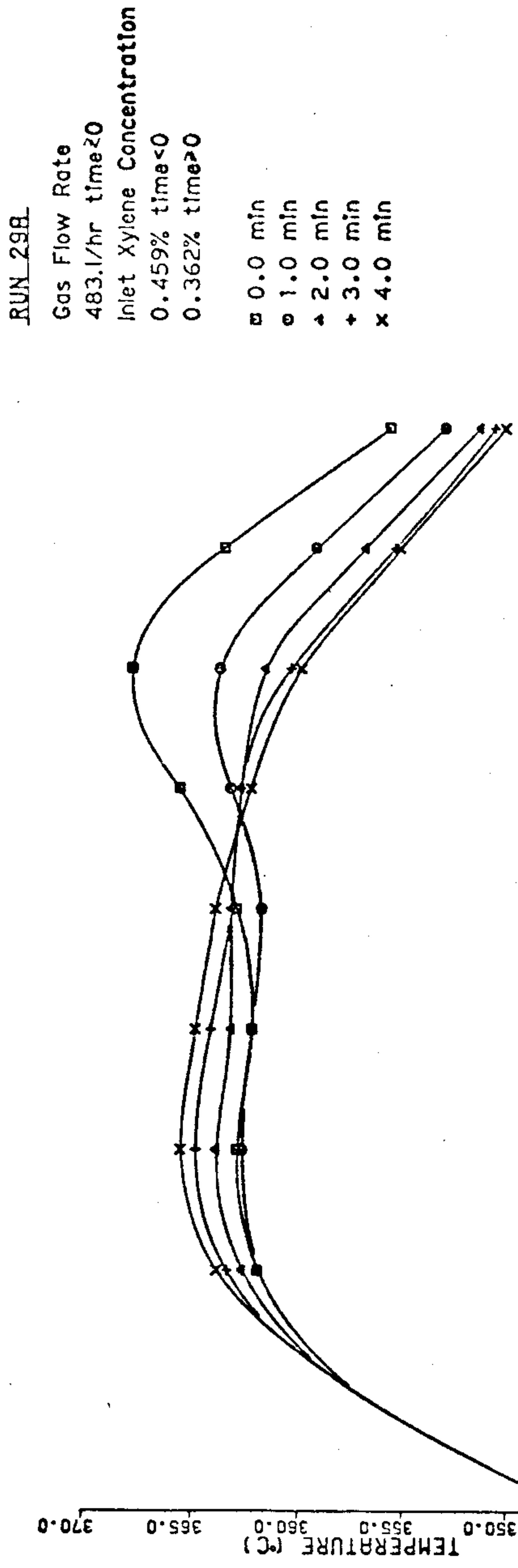
Although the axial temperature profiles were fitted satisfactorily by both the homogeneous and heterogeneous models, the extent of the reaction did not compare so favourably. For the homogeneous model 94 to 98% of the o-xylene reacted while for the heterogeneous model 91 to 96% reacted, compared with the average experimental value of 99.5%. In graphs 4.5 to 4.8 of the calculated axial temperature profiles, no consistent difference occurs between the two models. The decreased amount of reaction taking place in the heterogeneous model is due therefore to the slightly lower frequency factor and the slightly lower effective radial conductivity, obtained from the non-linear regression analysis.

Considering that the outlet o-xylene concentration was not included in the sum of squares for the regression analysis, the accuracy in modelling is satisfactory.

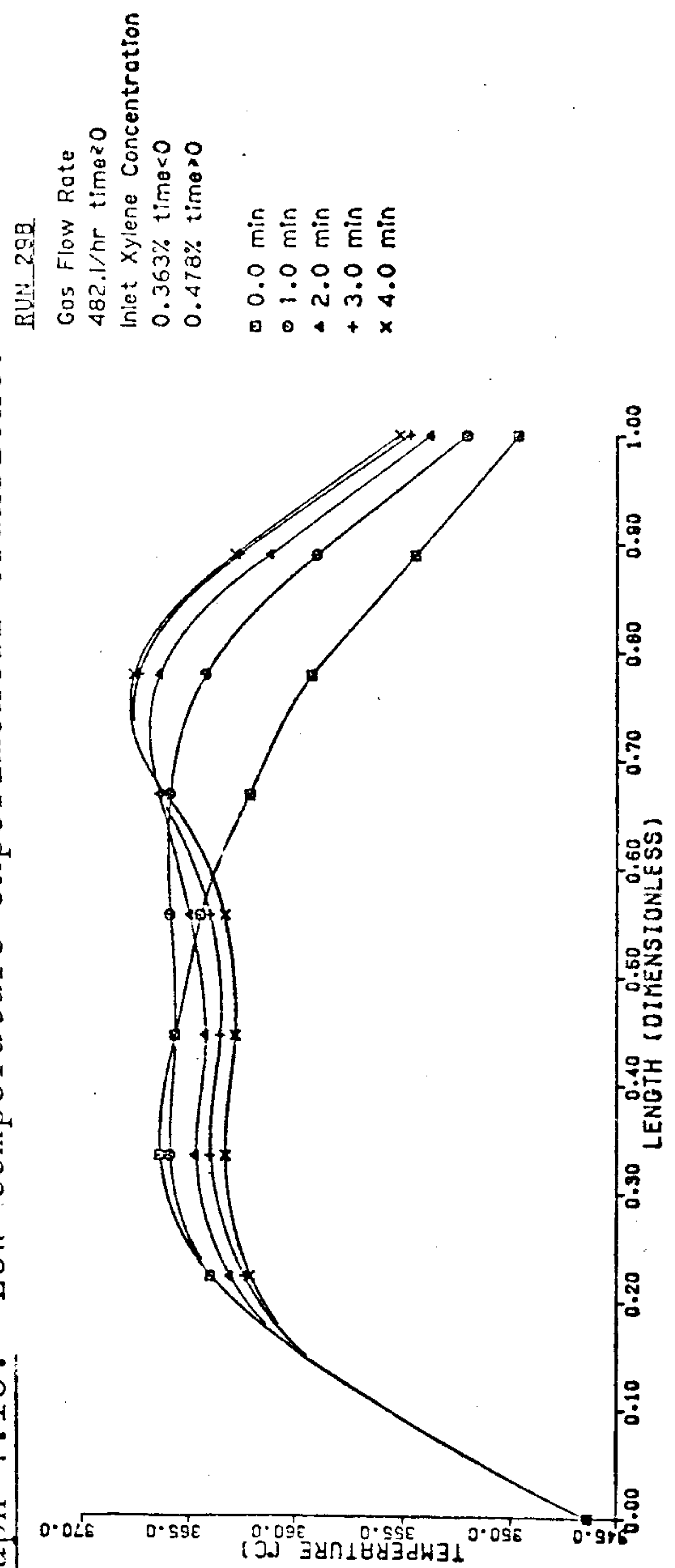
The use of an overall heat of reaction with only a single reaction taking place, implies that the heat of reaction is constant along the packed bed. This is very unlikely to be true. Improved accuracy in modelling the extent of the reaction may be achieved by employing a series reaction model, as this would lengthen the hot spot where most of the reaction occurs. As no intermediate concentrations along the bed were measured, no improvements on the present assumption can easily be made, except by drastically increasing the complexity of the non-linear regression analysis to consider a network of reactions. The limited data available makes such an alternative unfeasible.

4.4iii Low Conversion Runs

During start-up of the reactor, an unusual double hot spot was sometimes noticed. This generally occurred before the bath temperature was up to its normal operating value, with a correspondingly low conversion of o-xylene. A brief investigation of this phenomenon was carried out in runs 24 and 29, see graphs 4.10 and 4.11. The operating conditions were found to be completely stable and showed the anomalous behaviour already mentioned. To model a double hot spot, the reaction must occur by successive oxidation steps with the possible intermediates being o-tolualdehyde,



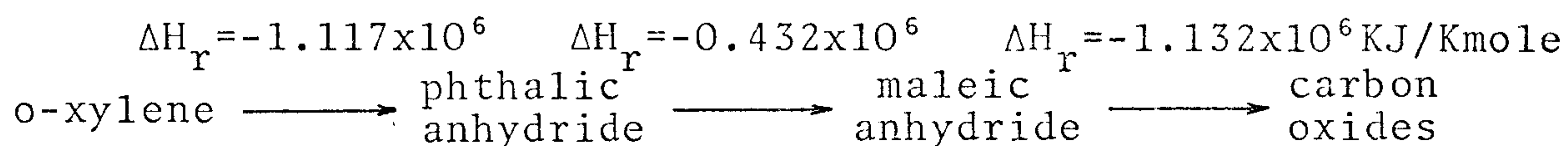
Graph 4.10. Low temperature experimental transient.



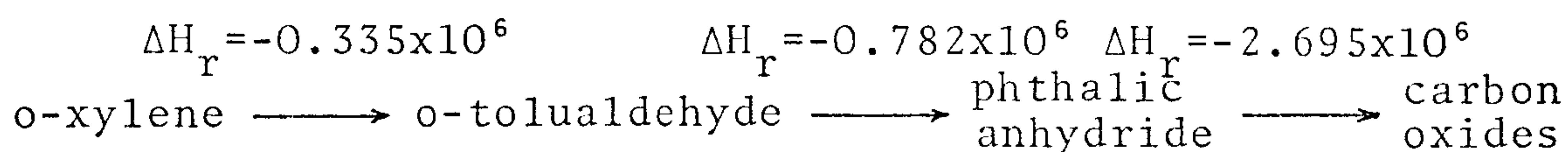
Graph 4.11. Low temperature experimental transient.

phthalide, phthalic anhydride and maleic anhydride. The typical product distribution was 65% phthalic anhydride, 18% carbon oxides with a CO_2/CO ratio of 3.0, 5% maleic anhydride or o-tolualdehyde, with the remainder being unreacted o-xylene. A trace of phthaldialdehyde and phthalide was normally detected. As not only the ratio of CO_2/CO , but also the ratio of carbon oxides to phthalic anhydride was slightly greater than for the higher temperature runs the overall heat of reaction was approximately 5% greater.

To obtain a double hot spot using only first order reactions there must be at least three series reactions. The heats of reactions may also be important so that the simplest probable model is



As can be seen, the heats of reaction are very amiable towards a double hot spot occurring. Another model tried was



The heats of reaction in this case are less likely to result in a double hump on the axial temperature profile.

The modelling of this system was carried out using a homogeneous model, two-dimensional in temperature but only one-dimensional in concentration. For both models, a double hot spot was achieved by non-linear regression of the 6 kinetic variables with the same heat transfer parameters as described previously for runs 19 and 21. The

maximum bed temperature however, was considerably higher than the experimental value and the second hot spot was not as convincing as that achieved experimentally. Due to the much higher bed temperatures, there was very little o-xylene left unreacted. The product distribution however did separate the two models with the first model containing the maleic anhydride being favoured. O-tolualdehyde cannot be completely eliminated as an intermediate as there may well be four reactions in a series.

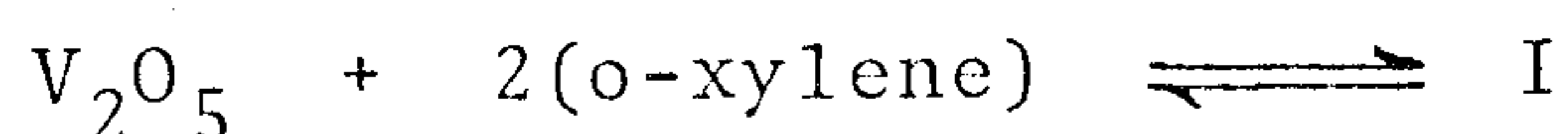
Although two first order exothermic reactions taking place in a non-adiabatic non-isothermal reactor cannot lead to a double hot spot, if the orders of the two reactors are different this phenomenon could well occur. For two reactions taking place by a bimolecular Langmuir-Hinshelwood model, with or without a summation term in the denominator, as proposed by Juusola (12) for the steady state adsorption model, a double hot spot may be possible. Use of the Langmuir-Hinshelwood or catalyst deactivation model would also explain the wrong way behaviour observed.

4.5 Dynamic Modelling

The dynamic model was solved, based on the values of the parameters obtained from the steady state heterogeneous non-linear regression analysis. Between the initial steady state and the final steady state, the effective overall heat of reaction (see appendix VII), and occasionally the frequency factor, as determined from the sum of squares minimisation varied, due to the varying selectivity of the

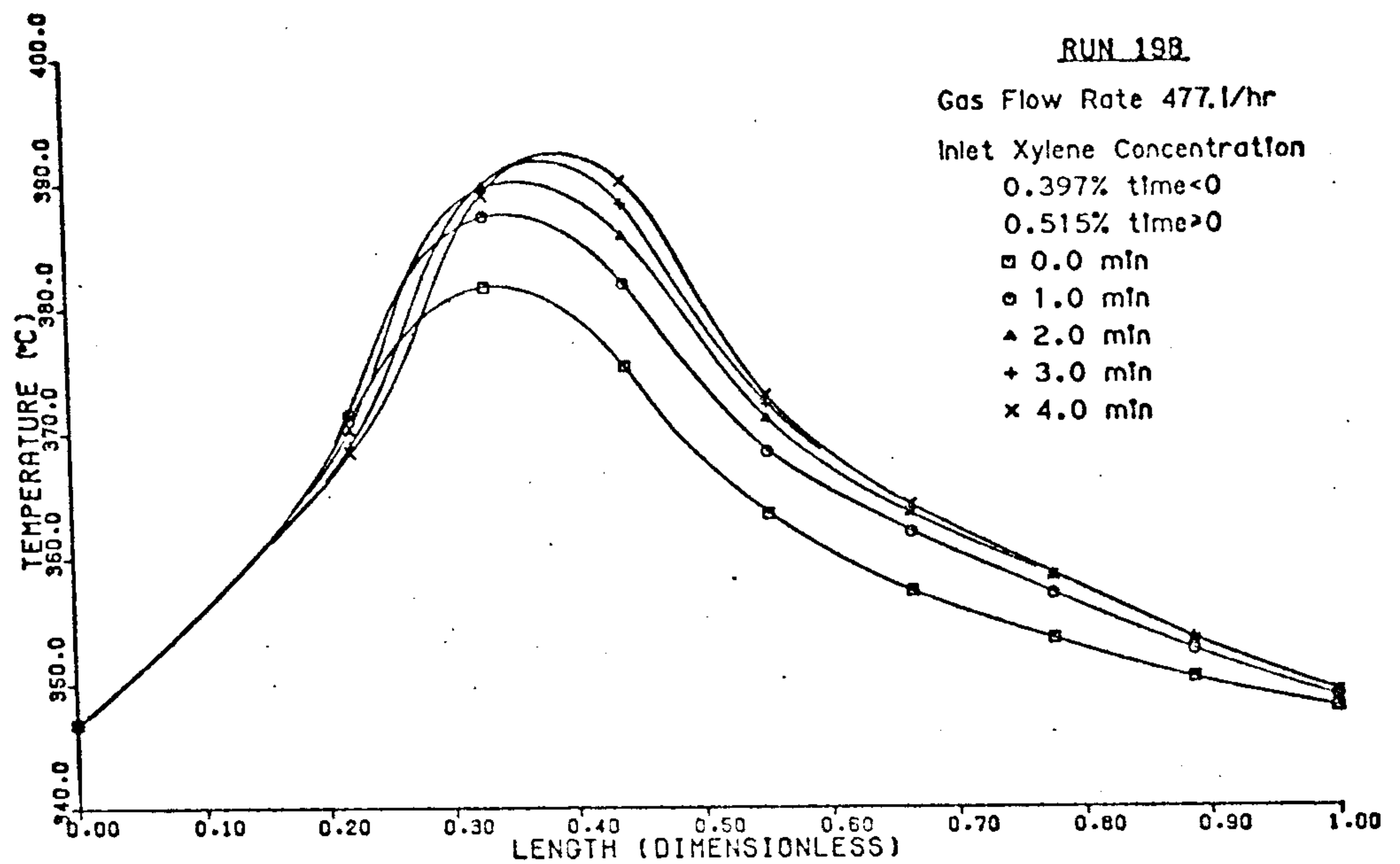
reaction. As only an overall rate of reaction was used, with no series or parallel reactions to account for selectivity variations, these effects were included in the transient model by linearly varying the frequency factor, and the heat of reaction over the first four minutes of the transient. Graphs 4.12 to 4.27 show the experimental axial temperature profiles during the dynamic state.

The catalyst deactivation reaction

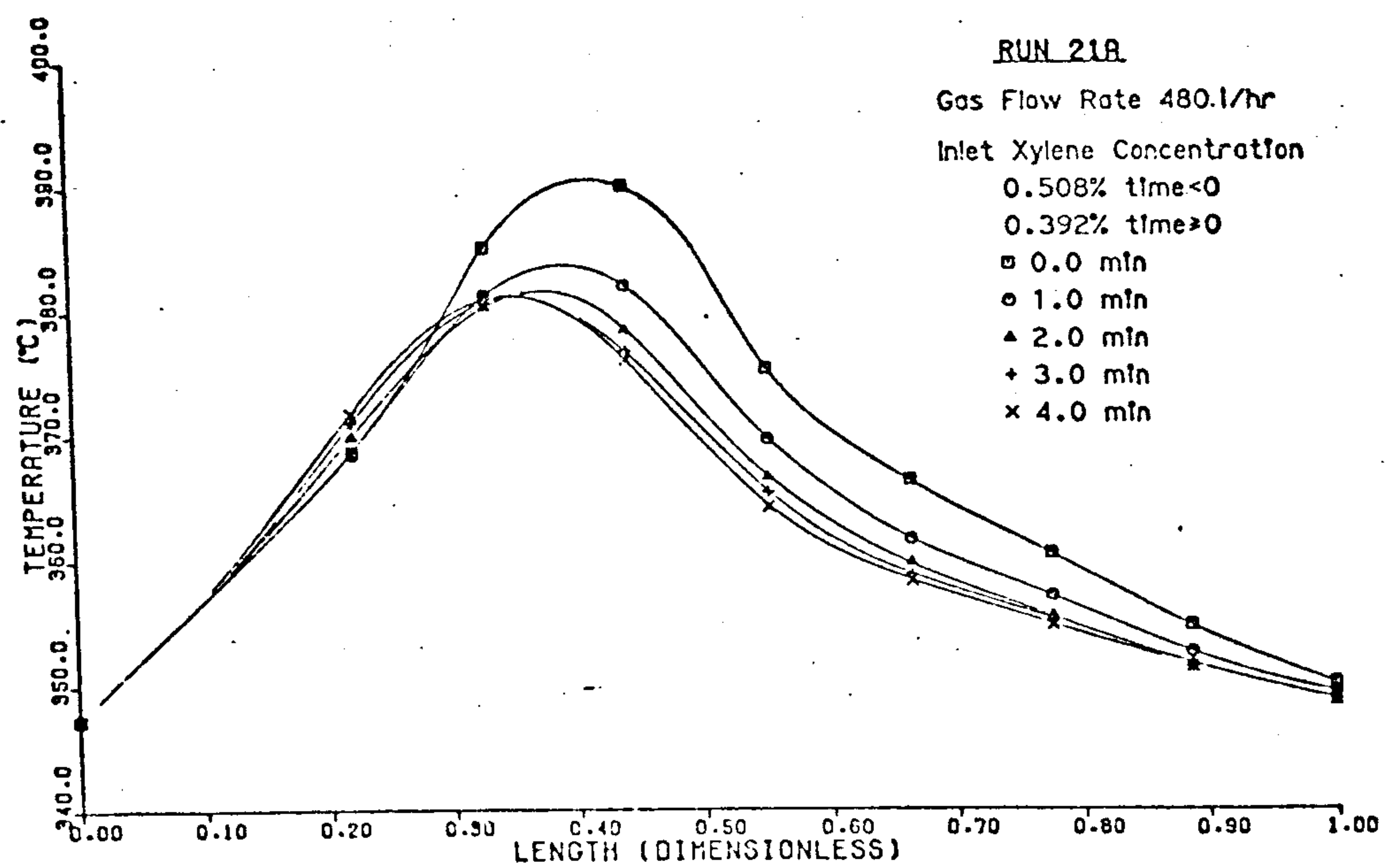


must be reversible, as no irreversible effects were found experimentally. The order of the two reactions was assumed to be zero with respect to the o-xylene concentration and first order with respect to either the active or inactive species. The rates of these reactions were expressed in terms of the reciprocals of the rate constants, the effective time constants.

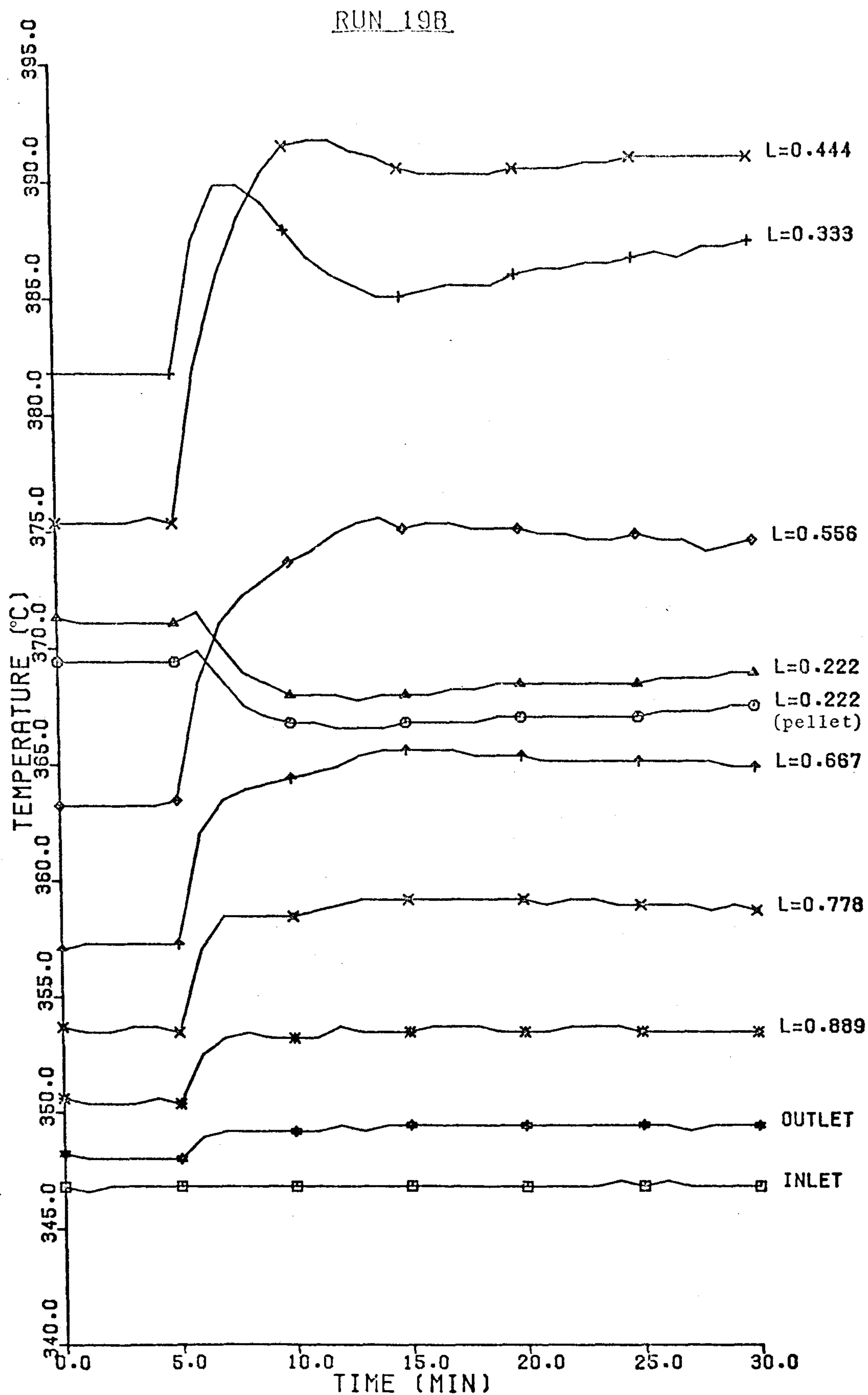
Solution of the full transient model including the transient concentration profiles proved not to be feasible as already mentioned in chapter 2.3, due to the large difference in the time constants of the energy and mass balance partial differential equations, giving rise to a "stiff" system. In an attempt to overcome this problem, the number of internal collocation points was increased to give a cubic approximation in the axial and time directions. This resulted in a marked improvement in the approximation of the step change, but no satisfactory convergence could be achieved. Rather than investigating the solution of



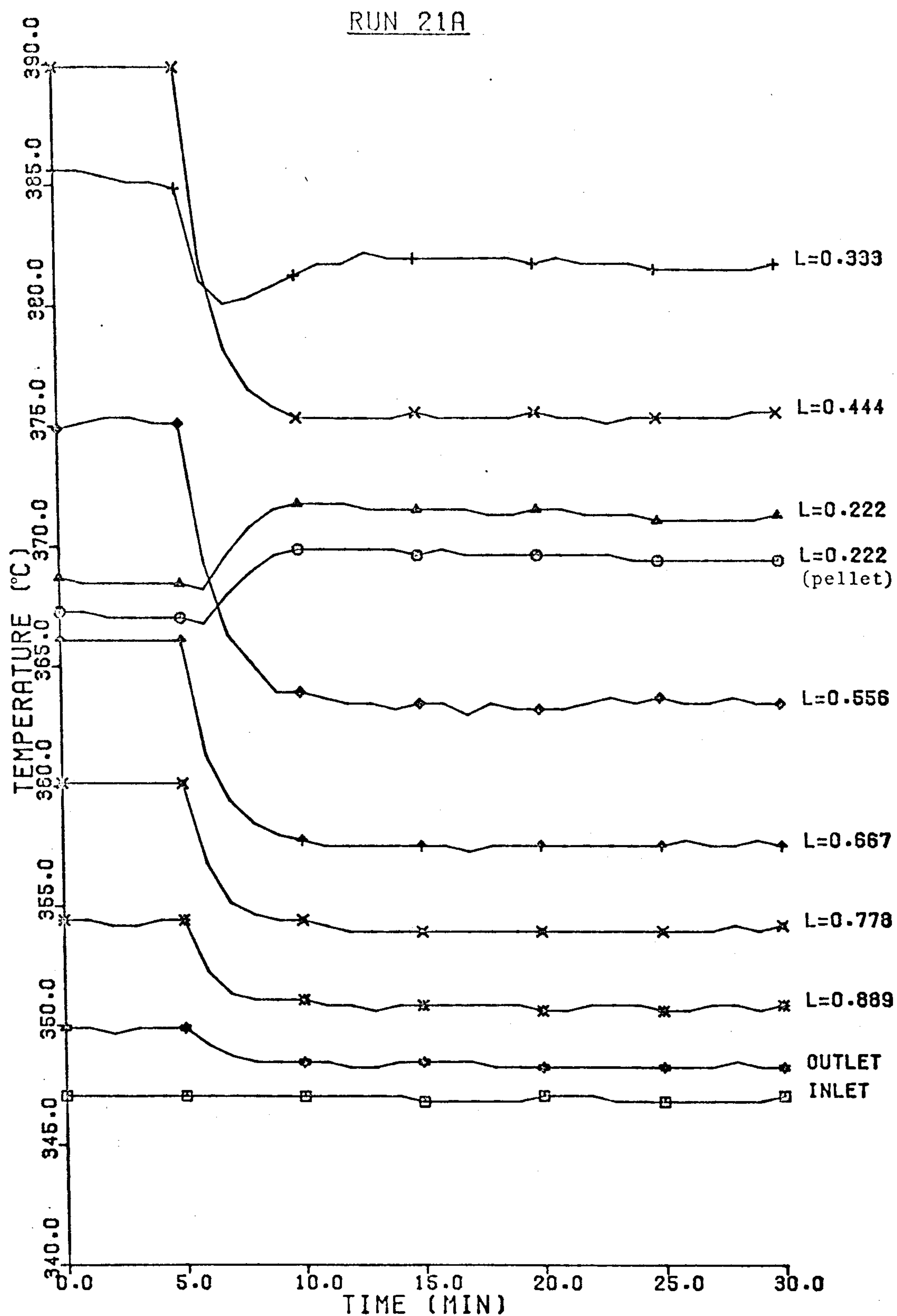
Graph 4.12. Experimental axial temperature profiles for an inlet xylene concentration step increase.



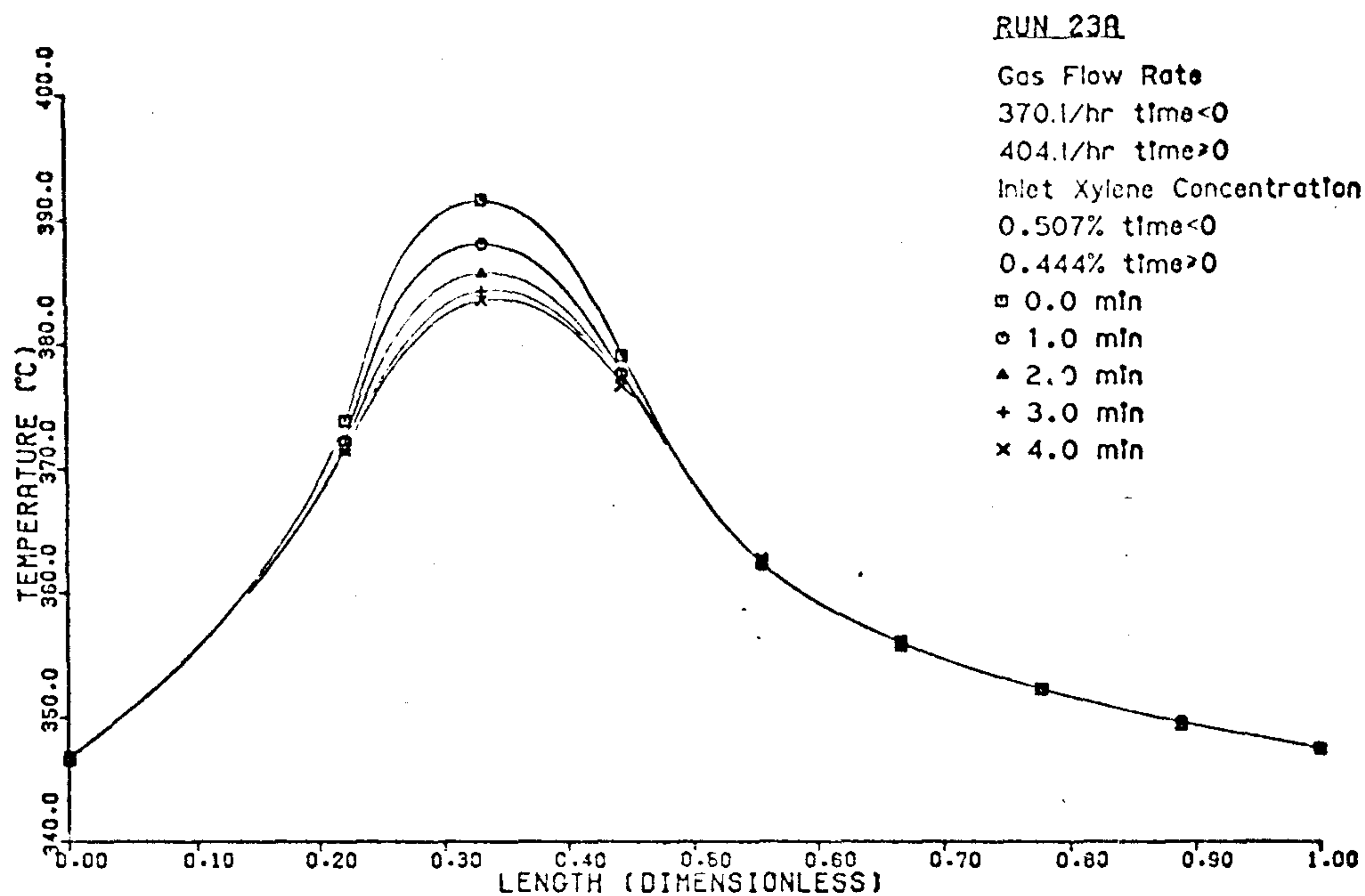
Graph 4.13. Experimental axial temperature profiles for an inlet xylene concentration step decrease.



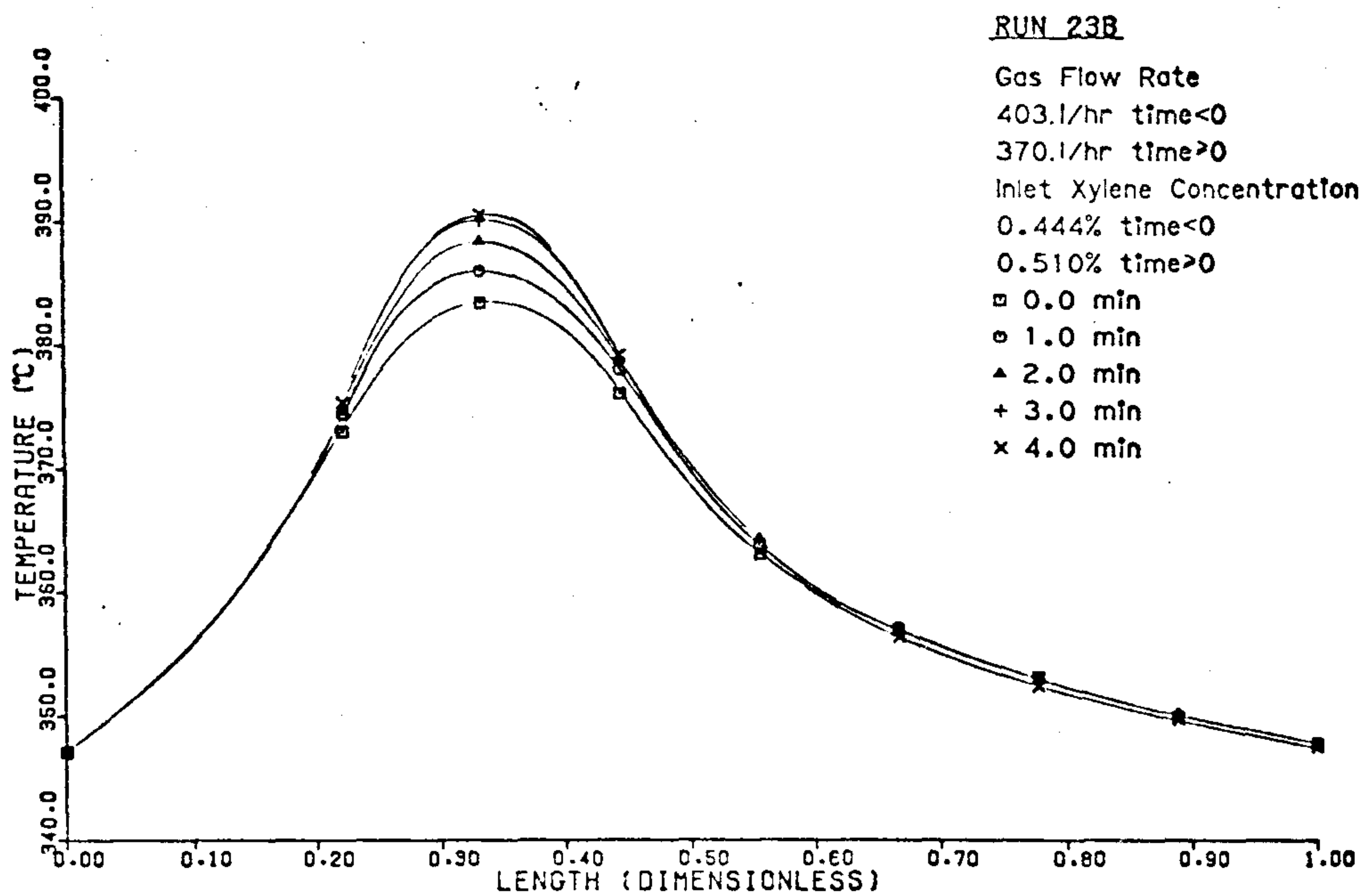
Graph 4.14. Experimental transient for an inlet xylene concentration step increase.



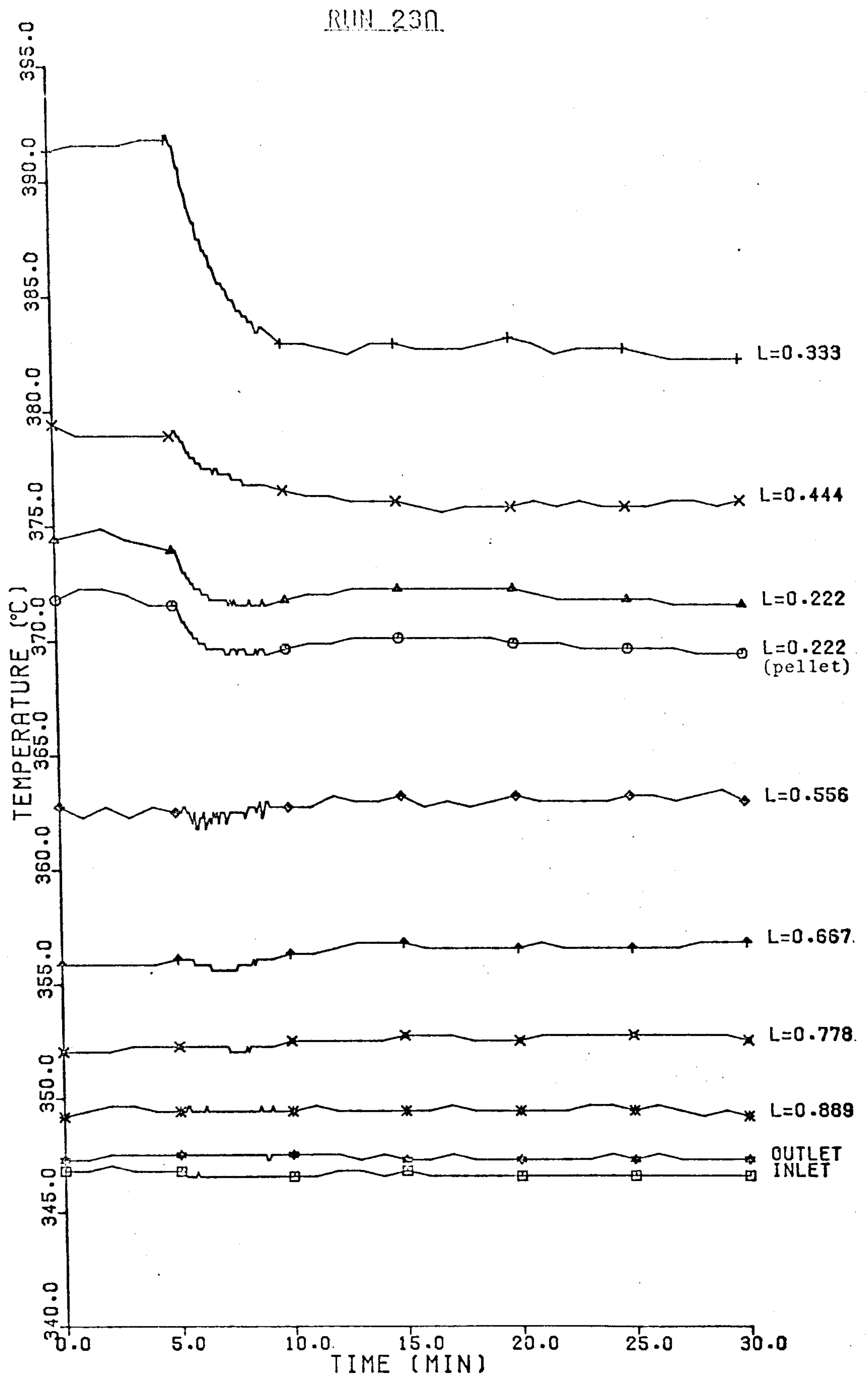
Graph 4.15. Experimental transient for an inlet xylene concentration step decrease.



Graph 4.16. Experimental transient for a xylene concentration step decrease and a gas rate step increase.

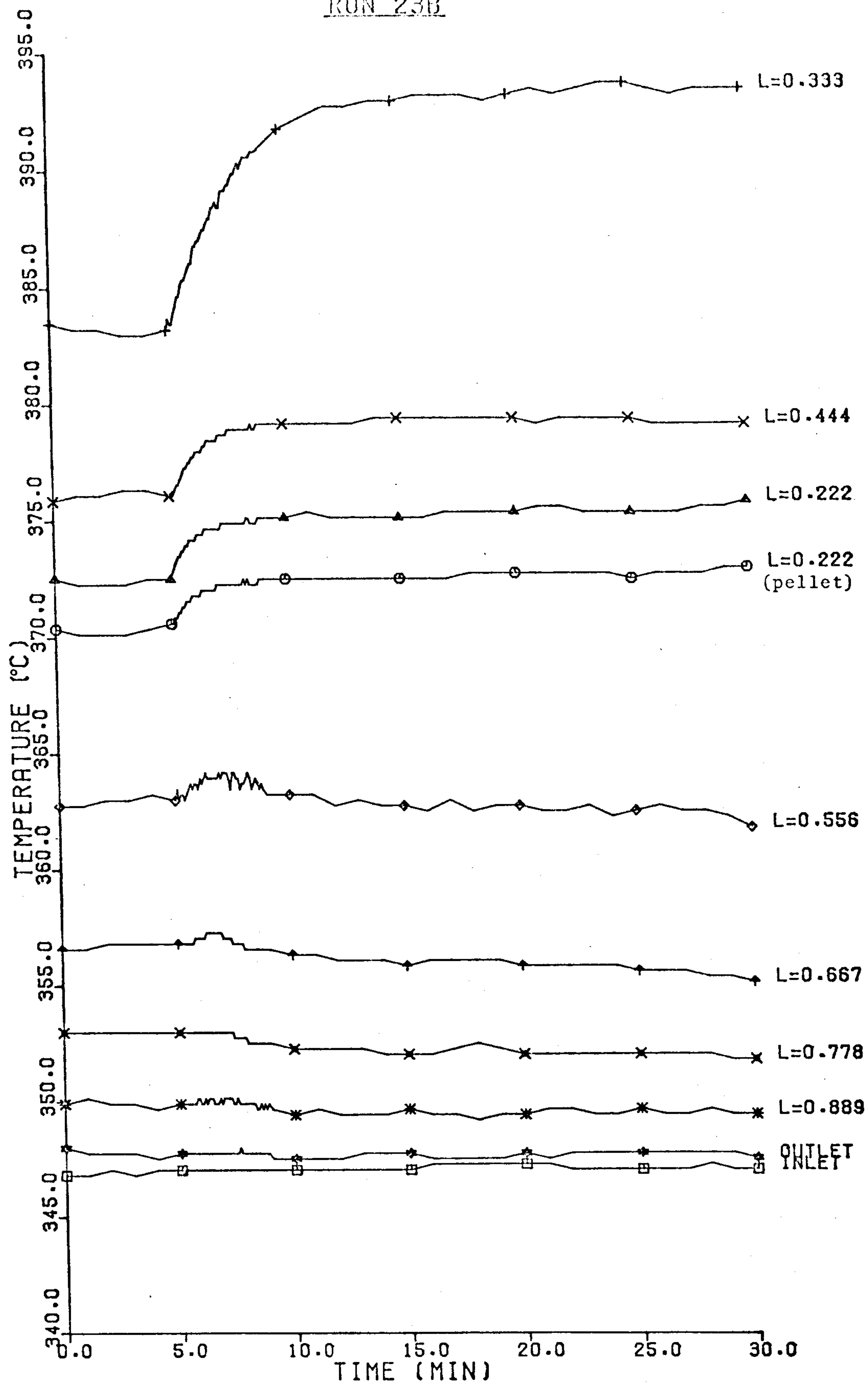


Graph 4.17. Experimental transient for a xylene concentration step increase and a gas rate step decrease.

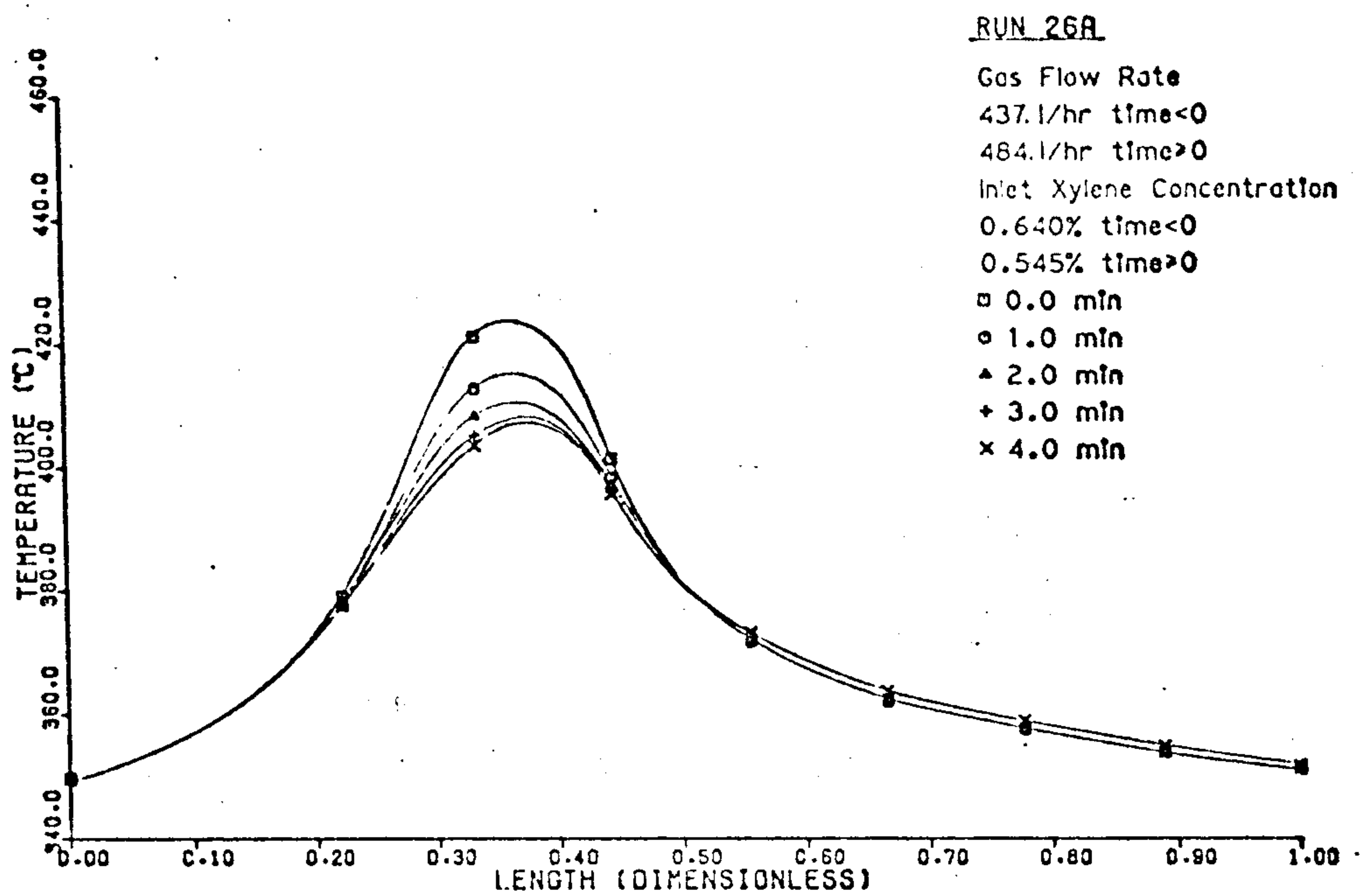


Graph 4.18. Experimental transient for a xylene concentration step decrease and a gas rate step increase.

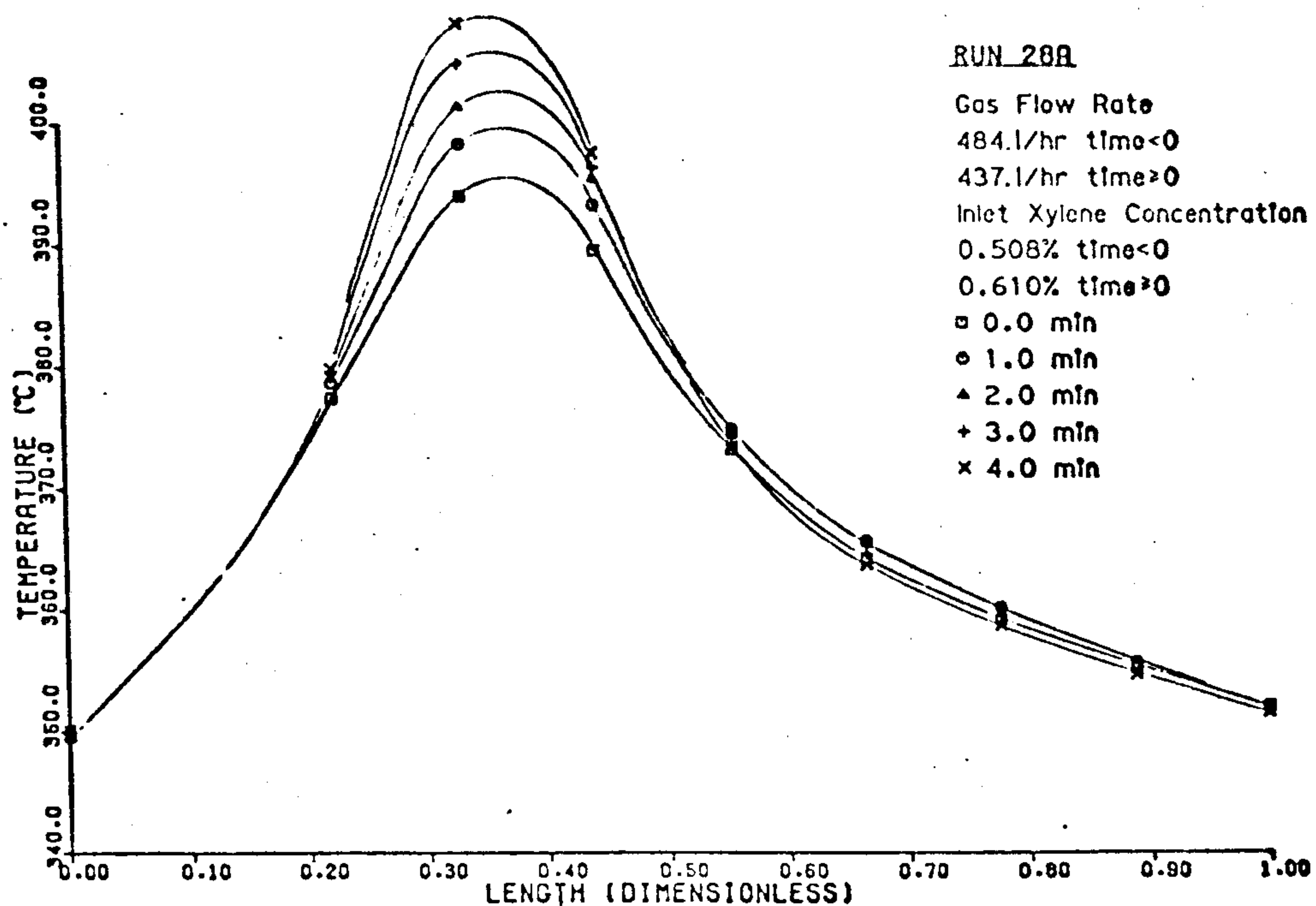
RUN 23B



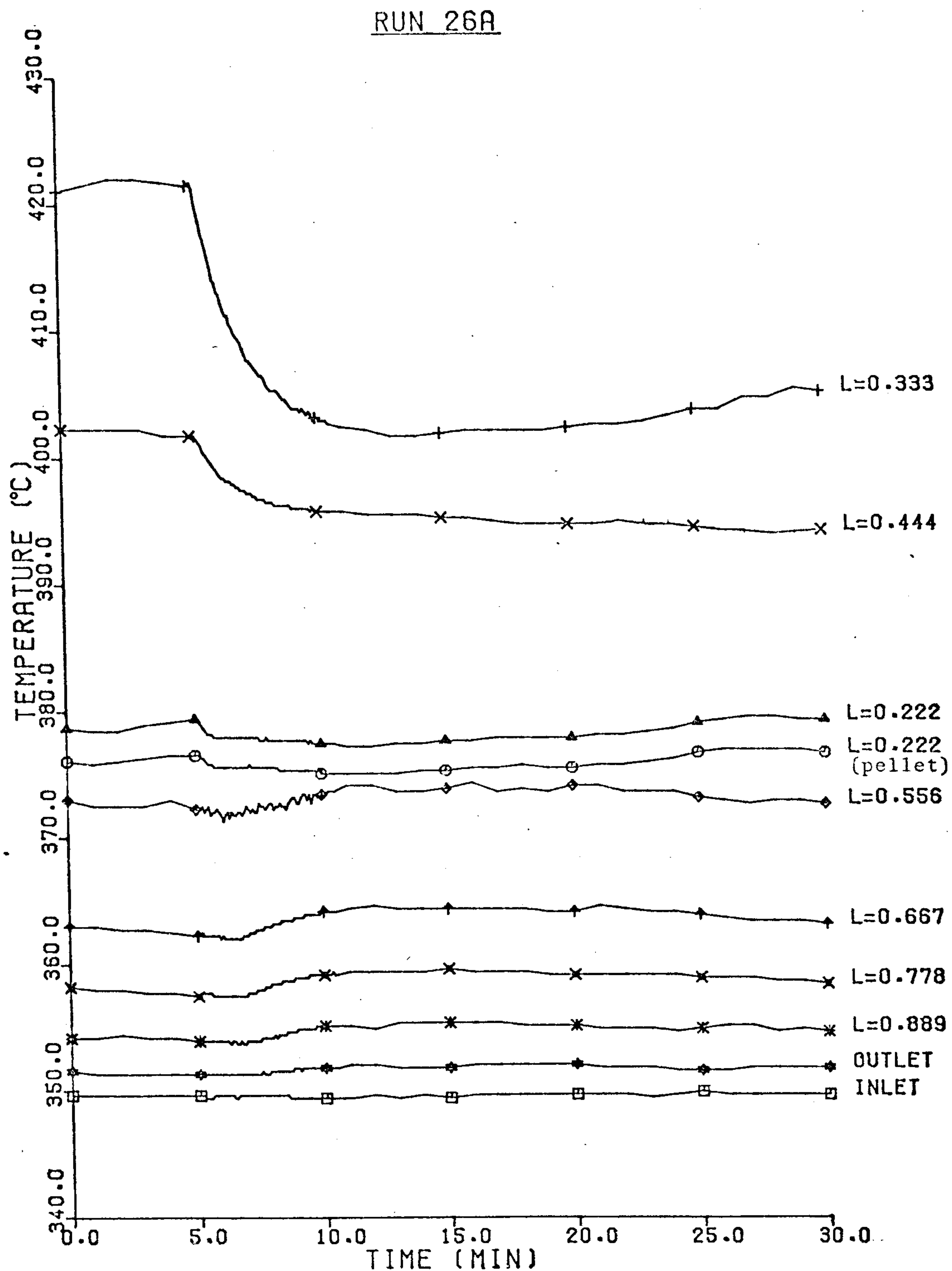
Graph 4.19. Experimental transient for a xylene concentration step increase and a gas rate step decrease.



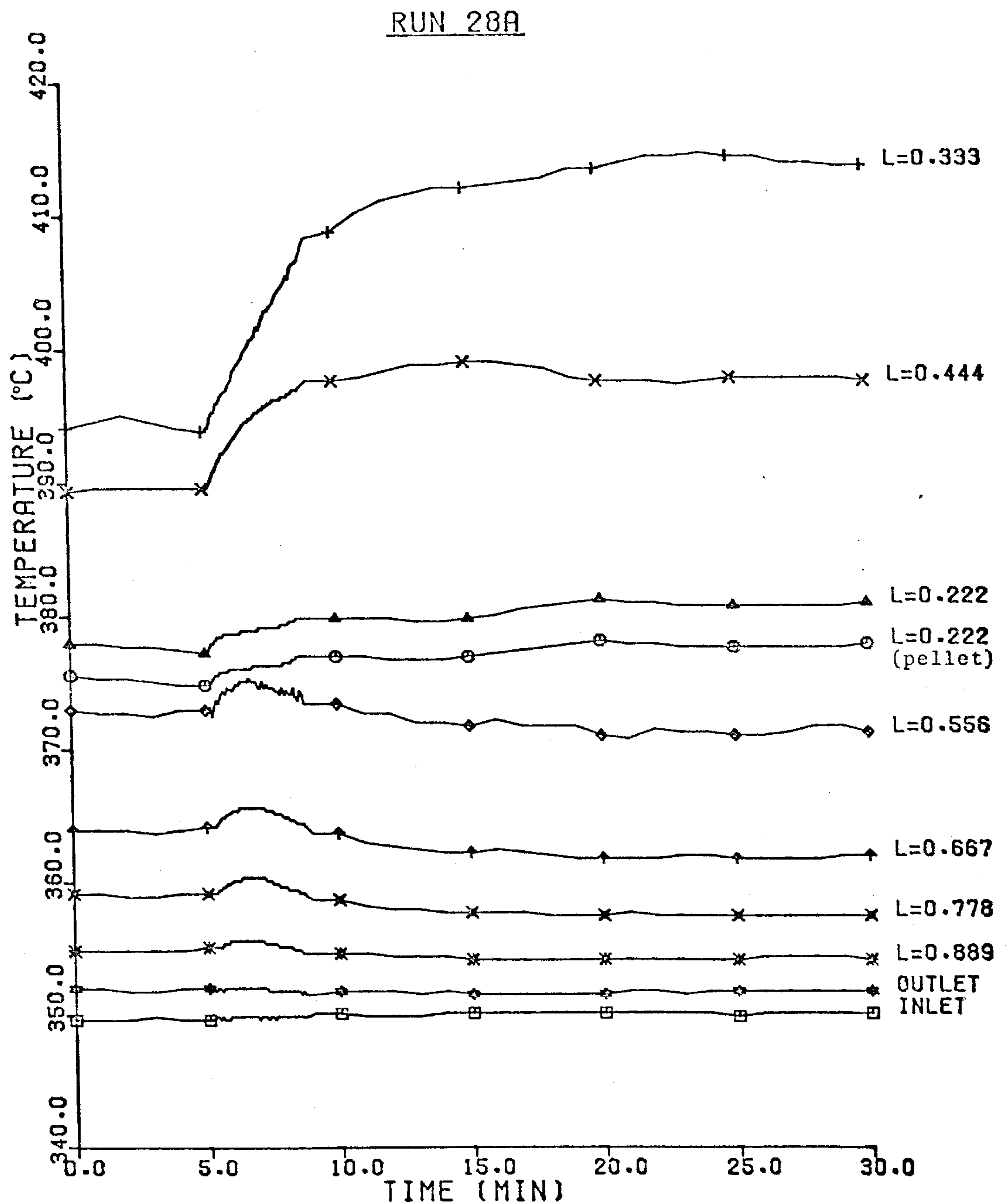
Graph 4.20. Experimental transient for a xylene concentration step decrease and a gas rate step increase.



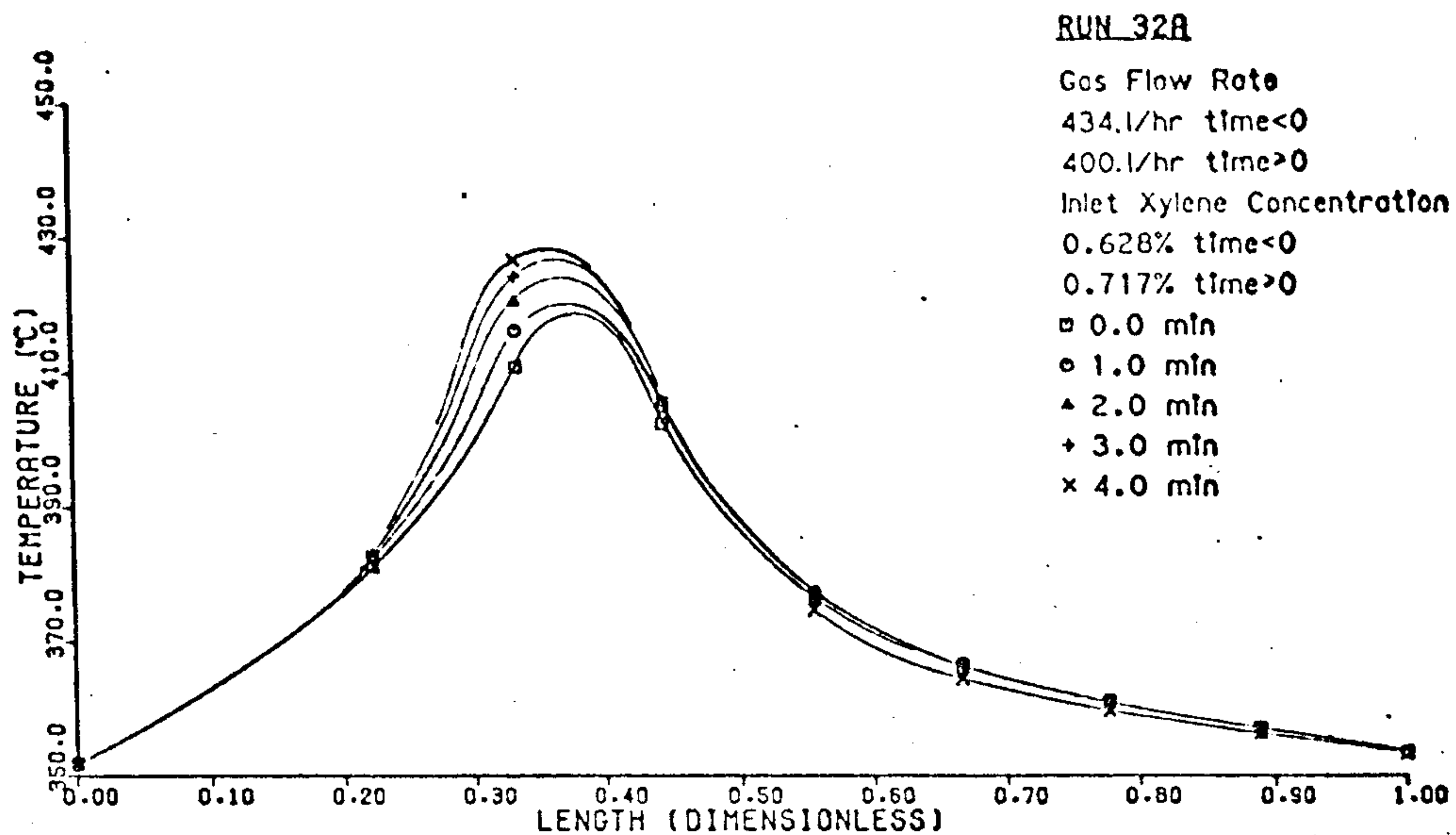
Graph 4.21. Experimental transient for a xylene concentration step increase and a gas rate step decrease.



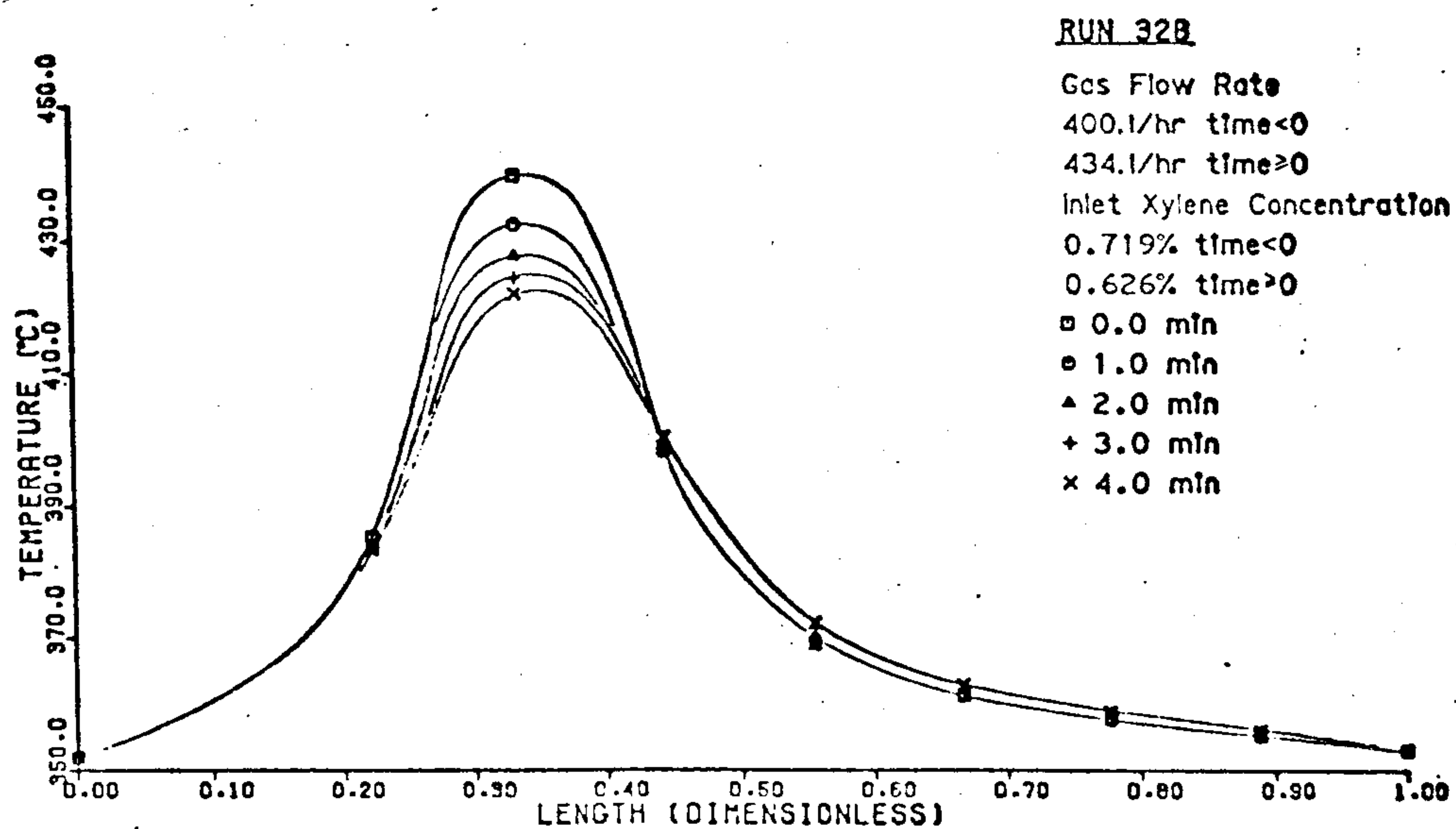
Graph 4.22. Experimental transient for a xylene concentration step decrease and a gas rate step increase.



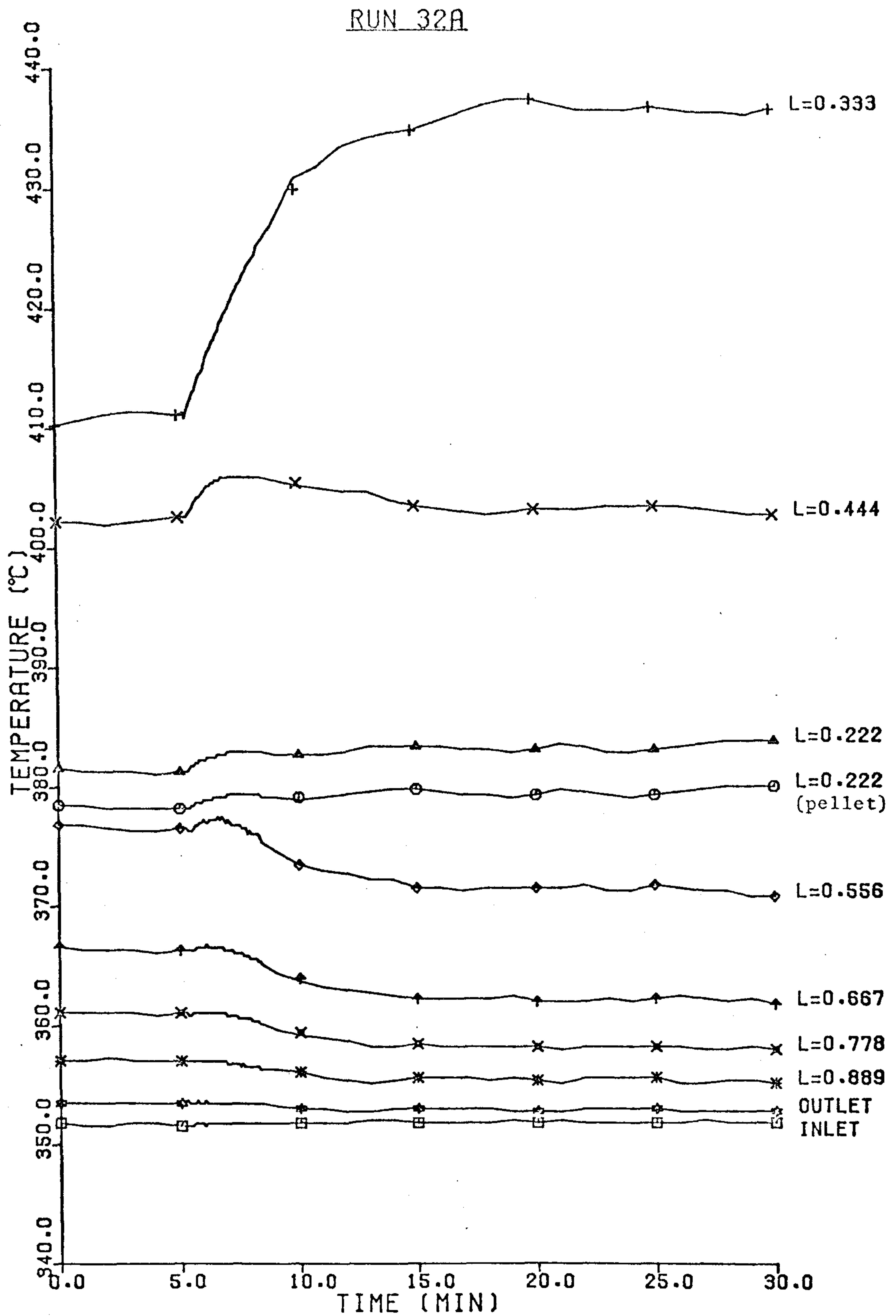
Graph 4.23. Experimental transient for a xylene concentration step increase and a gas rate step decrease.



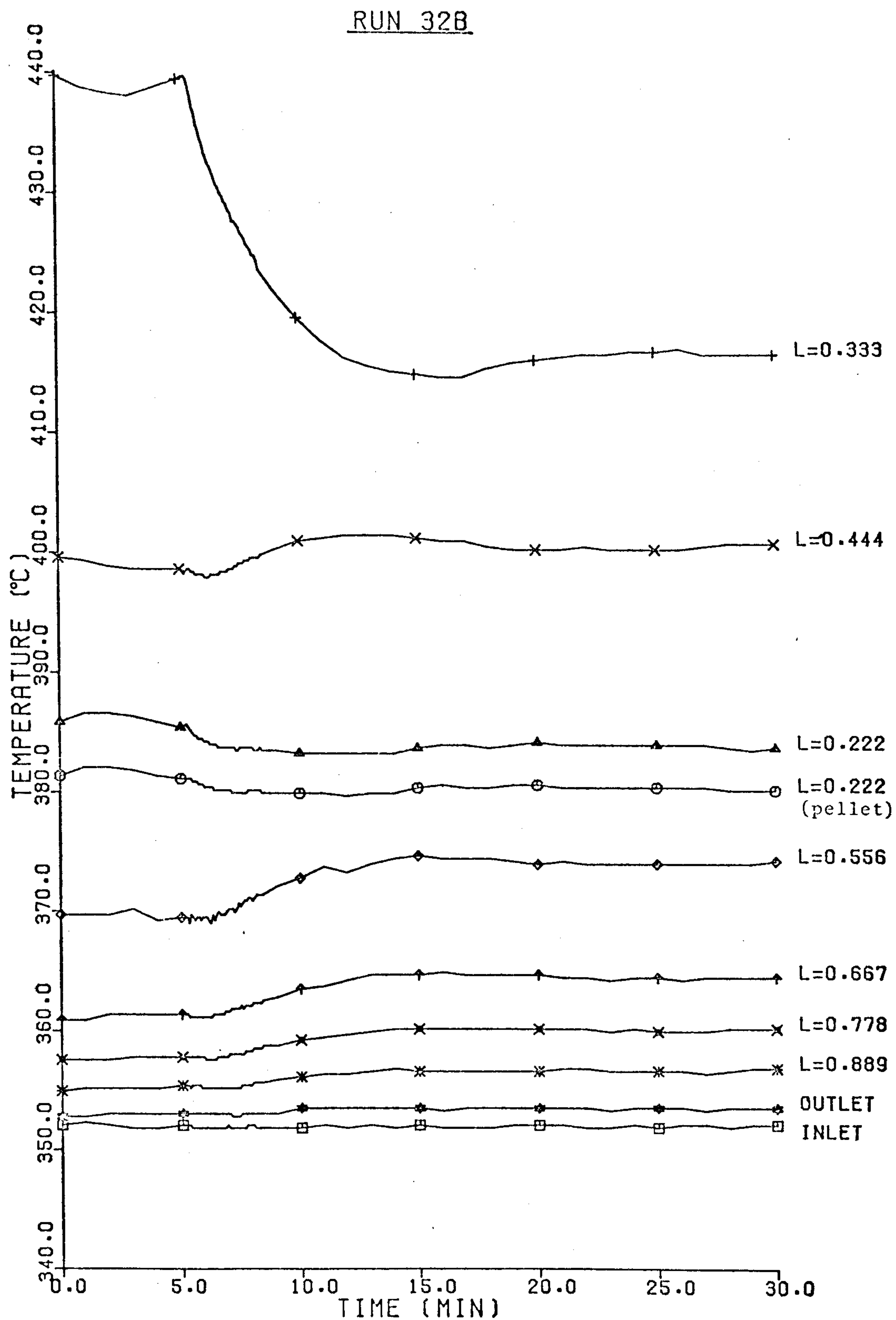
Graph 4.24. Experimental transient for a xylene concentration step increase and a gas rate step decrease.



Graph 4.25. Experimental transient for a xylene concentration step decrease and a gas rate step increase.



Graph 4.26. Experimental transient for a xylene concentration step increase and a gas rate step decrease.



Graph 4.27. Experimental transient for a xylene concentration step decrease and a gas rate step increase.

stiff sets of equations, further study was limited to the temperature transients with the concentration profiles going through a series of pseudo-steady states.

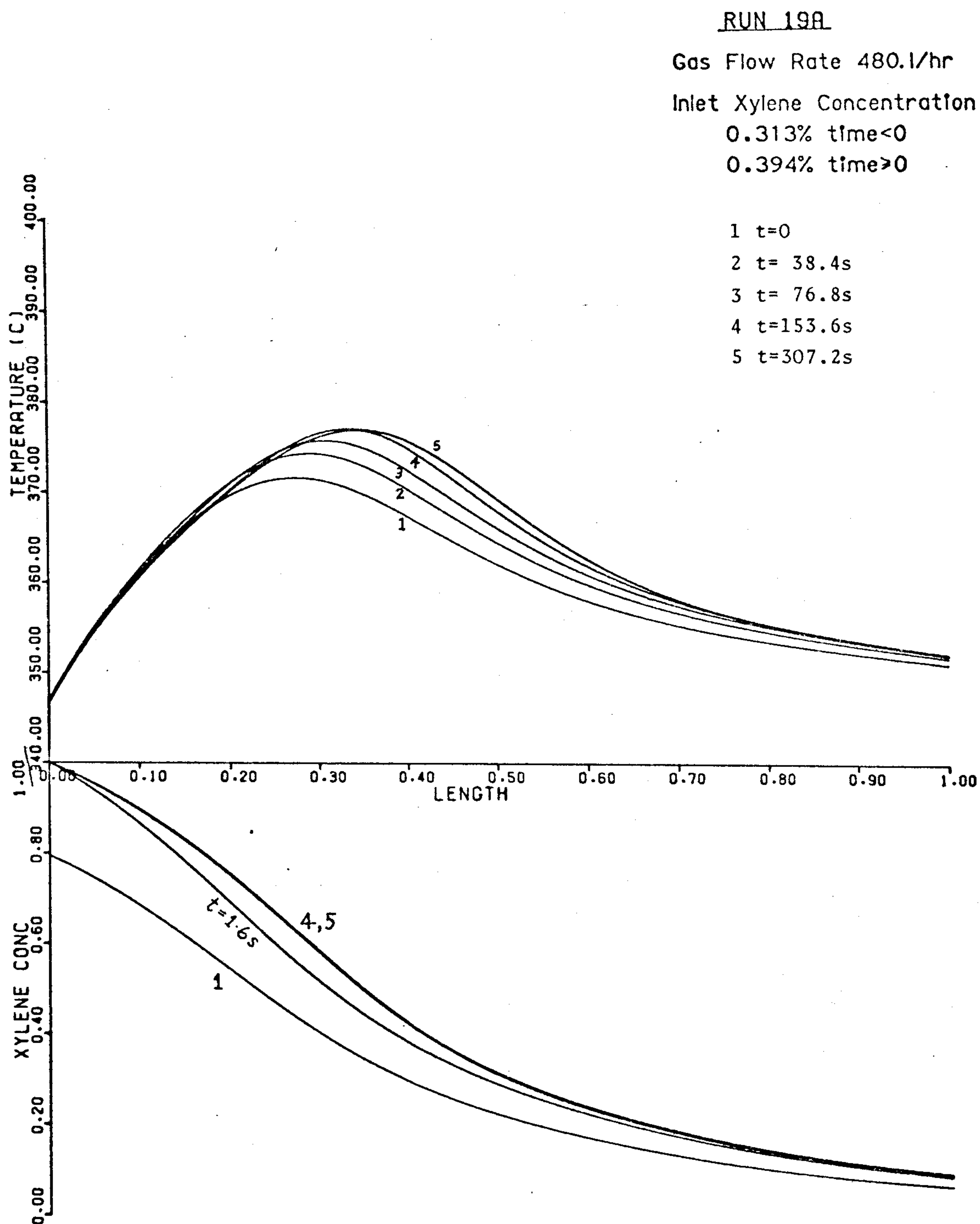
The solution of a normal first order catalytic reaction taking place in a packed bed under dynamic conditions can be solved assuming pseudo-steady state concentration profiles in steps of 20 seconds, which easily oversteps the discontinuity in the concentration and takes approximately 300 seconds of CDC 6400 computer time. In all cases, two internal radial collocation points with one internal collocation point in the axial and time directions were used, except for a brief satisfactory convergence check with four internal radial points.

Introducing the catalyst deactivation reaction can drastically increase the computing time, especially if the time constant for the catalyst deactivation reaction is decreased to 10 seconds. The pseudo-time constant of the reactor temperature itself is now very different from that of the catalyst deactivation reaction so that the system has almost reverted to the stiff set of equations of the full transient model. To maintain accuracy, the step size in the time direction must be decreased. For a final steady state average accuracy of $\pm 2^{\circ}\text{C}$ it was necessary to have a maximum step size of 0.80 seconds. This is still greater than the residence time of 0.2 seconds; however the time step is now in the range where it is necessary to consider the full transient model with the dynamic concentration profile. This was not done, due to the complexity

of the problem and the computing time necessary. To save computer time, for some of the runs with a 10 second catalyst deactivation time constant, only the more interesting first half of the reactor has been modelled. Graphs 4.28, 30, 33, and 35, show the variation of the temperature and concentration profiles of the model under dynamic conditions. These transients are compared with the experimental transients in graphs 4.29, 31, 32, 34, and 36.

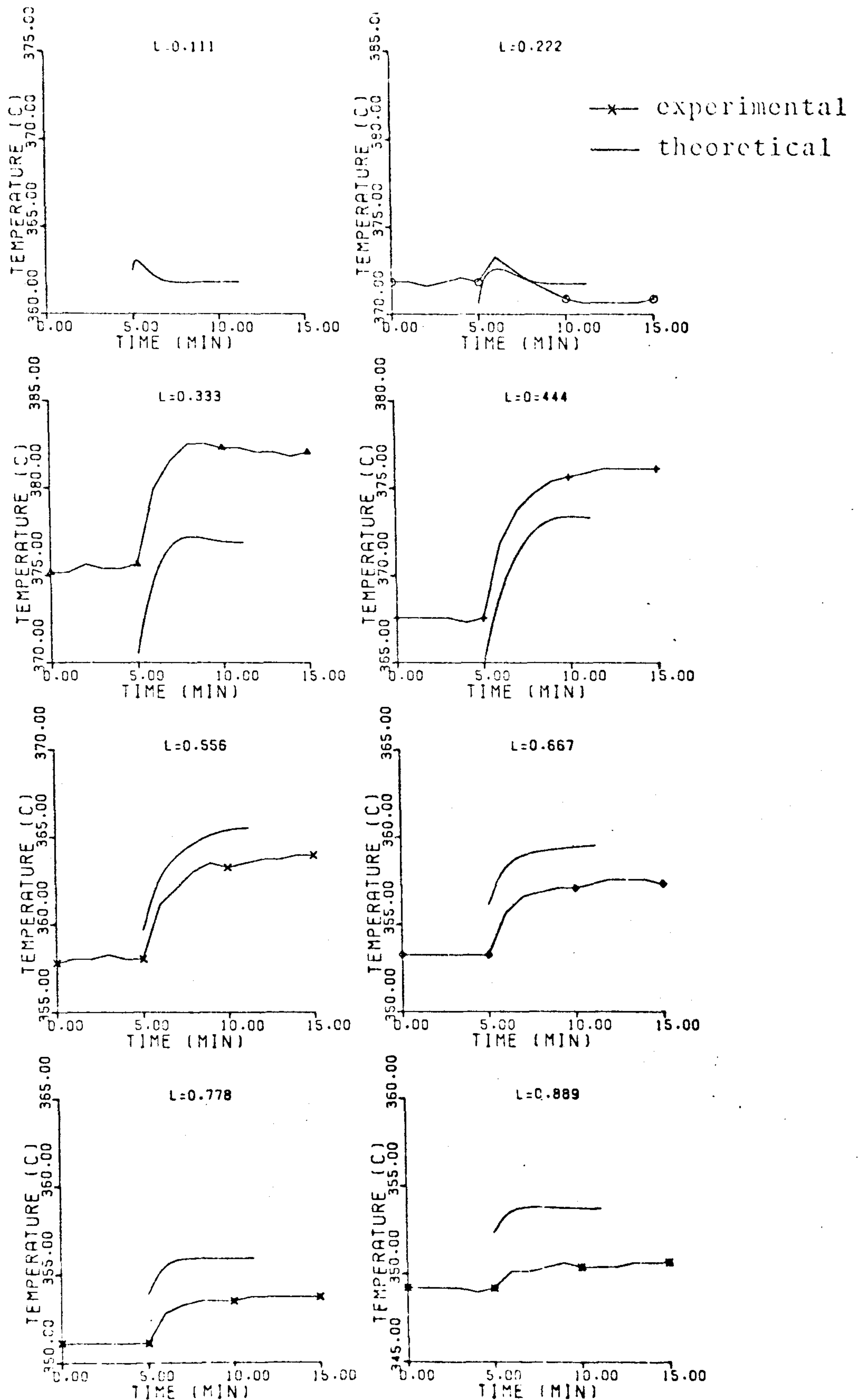
Up to a dimensionless length of 0.25, the effect of decreasing the time constant for the catalyst deactivation reaction is to decrease the initial amount of "right way" movement of the temperature so that the "wrong way" movement occurs earlier. For the dimensionless length between 0.25 and 0.50, decreasing the time constant decreases the amount of overshoot of the final steady state. Over the last half of the reactor, variation of the time constant of the catalyst deactivation reaction has very little effect.

As can be seen from graphs 4.29 and 32, solution of the catalyst deactivation model under dynamic conditions when the inlet o-xylene concentration is increased at a constant gas flow rate, leads to initial right way behaviour for the first part of the reactor followed by wrong way behaviour to a new steady state at a lower temperature. The reverse concentration change is shown in graphs 4.31, 34, and 36. The excessive amount of wrong way behaviour occurring in the dynamic modelling at high o-xylene concentration (as $t \rightarrow \infty$) is due to the large amount of error,

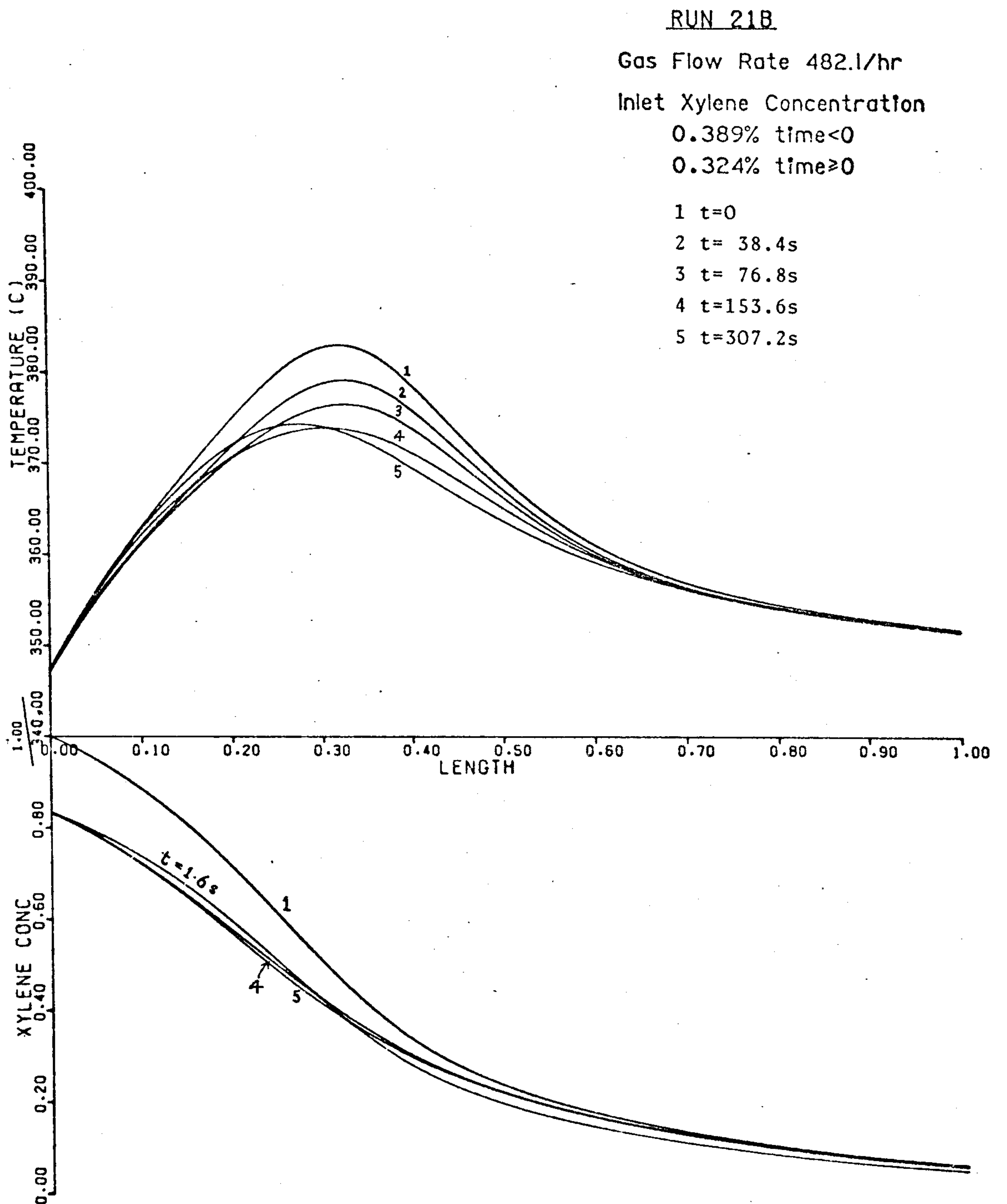


Graph 4.28. Theoretical axial temperature and concentration profiles for a xylene concentration step increase.

RUN 19A

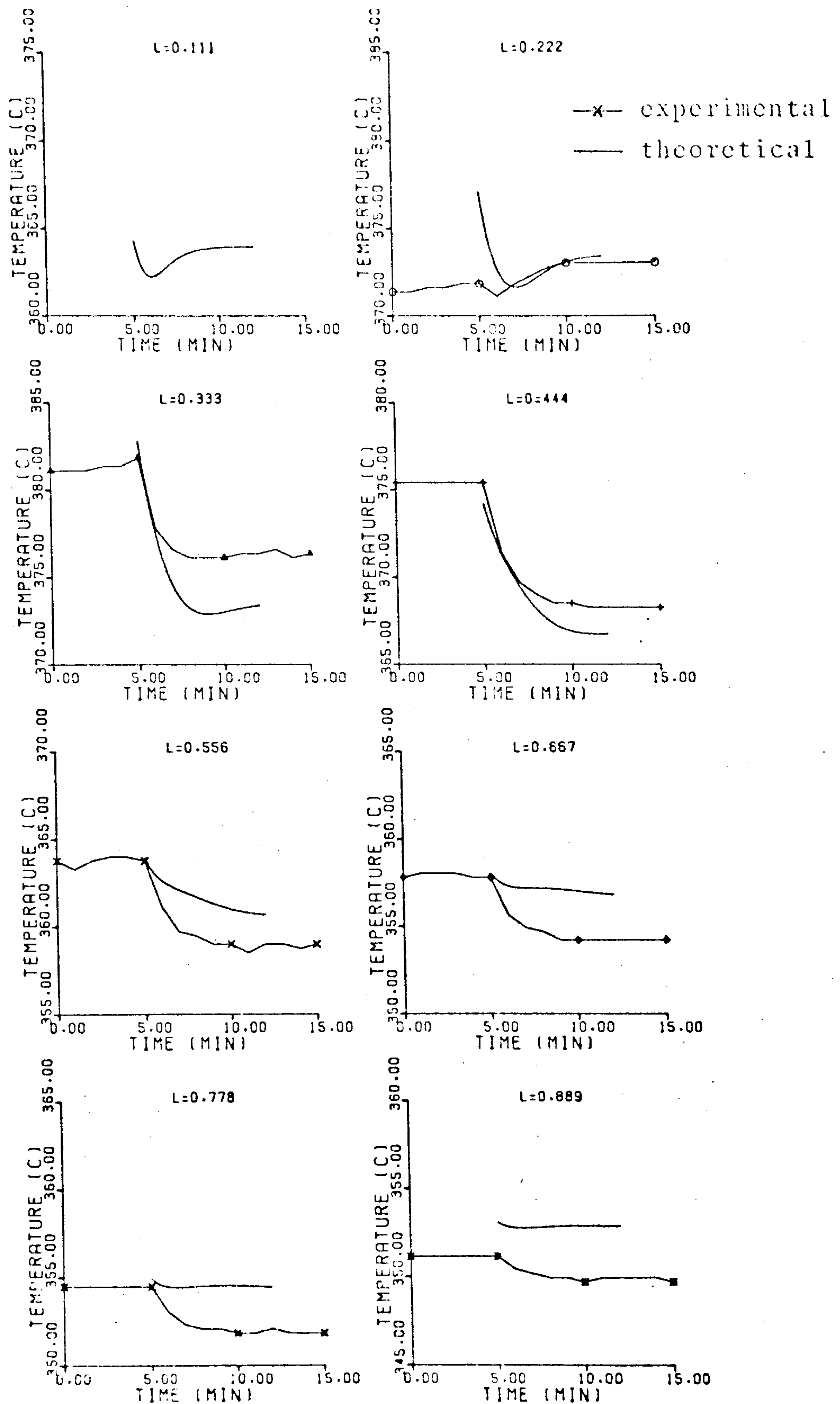


Graph 4.29. Theoretical and experimental axial temperatures for a xylene concentration step increase.



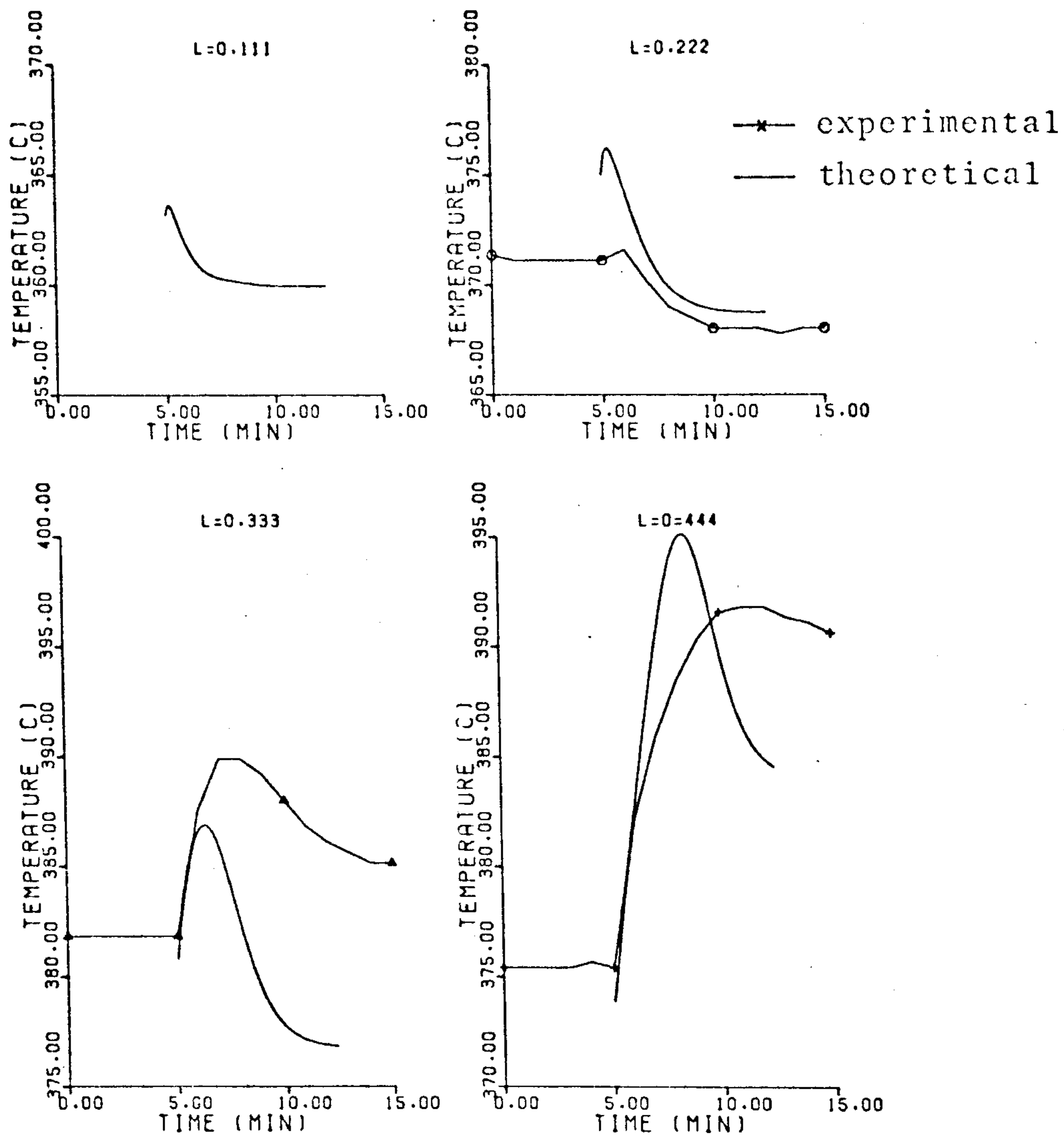
Graph 4.30. Theoretical axial temperature and concentration profiles for a xylene concentration step decrease.

RUN 21B

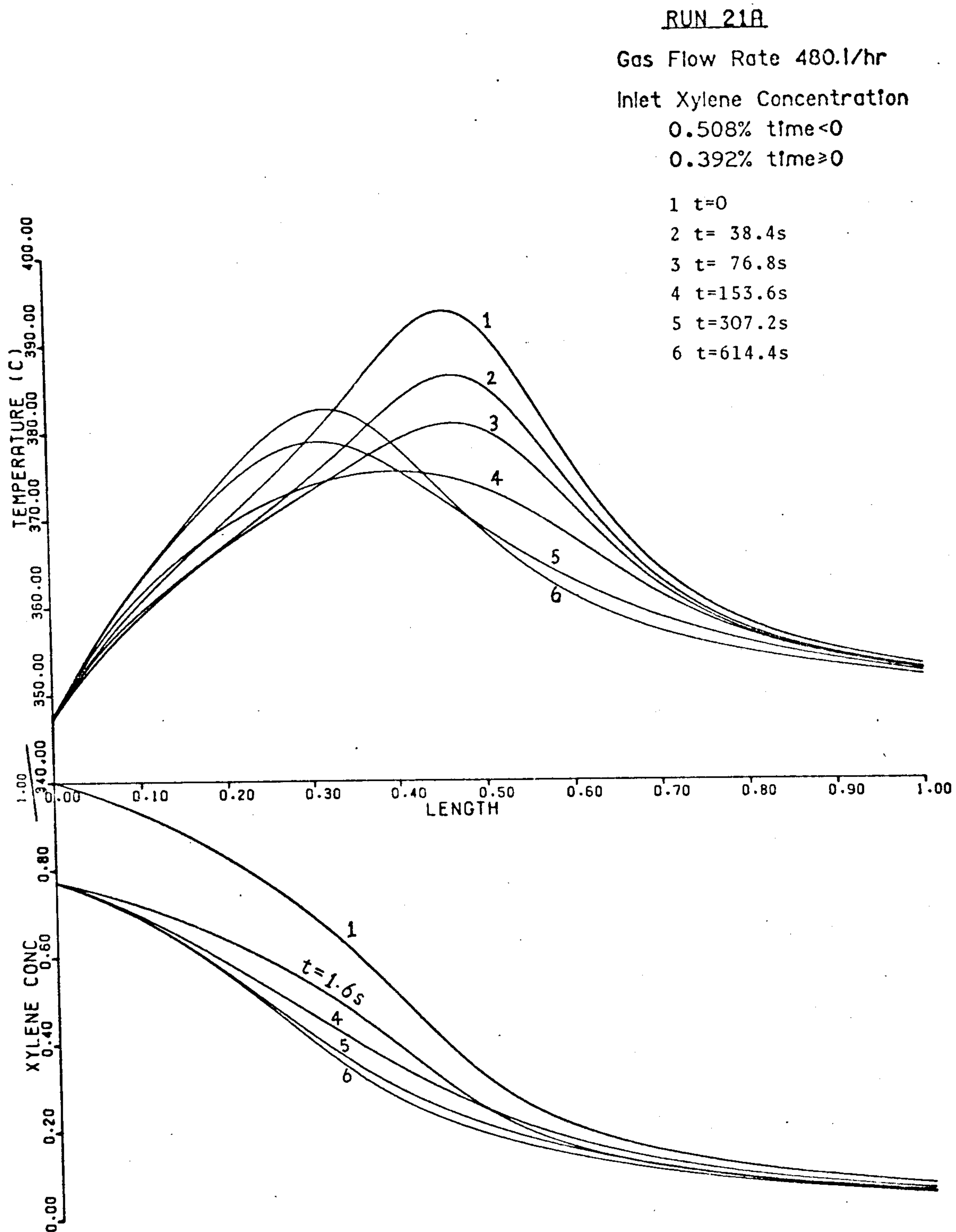


Graph 4.31. Theoretical and experimental axial temperatures for a xylene concentration step decrease.

RUN 19B

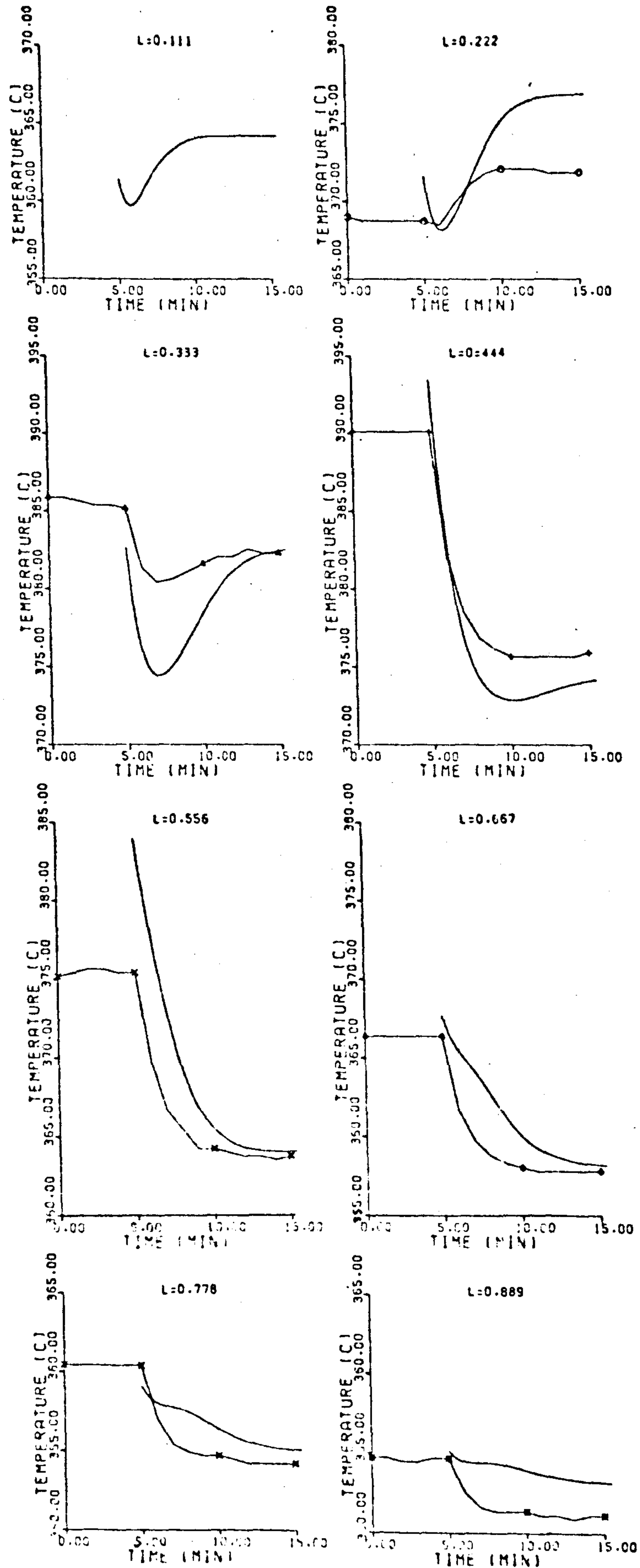


Graph 4.32. Theoretical and experimental axial temperatures for a xylene concentration step increase.



Graph 4.33. Theoretical axial temperature and concentration profiles for a xylene concentration step decrease.

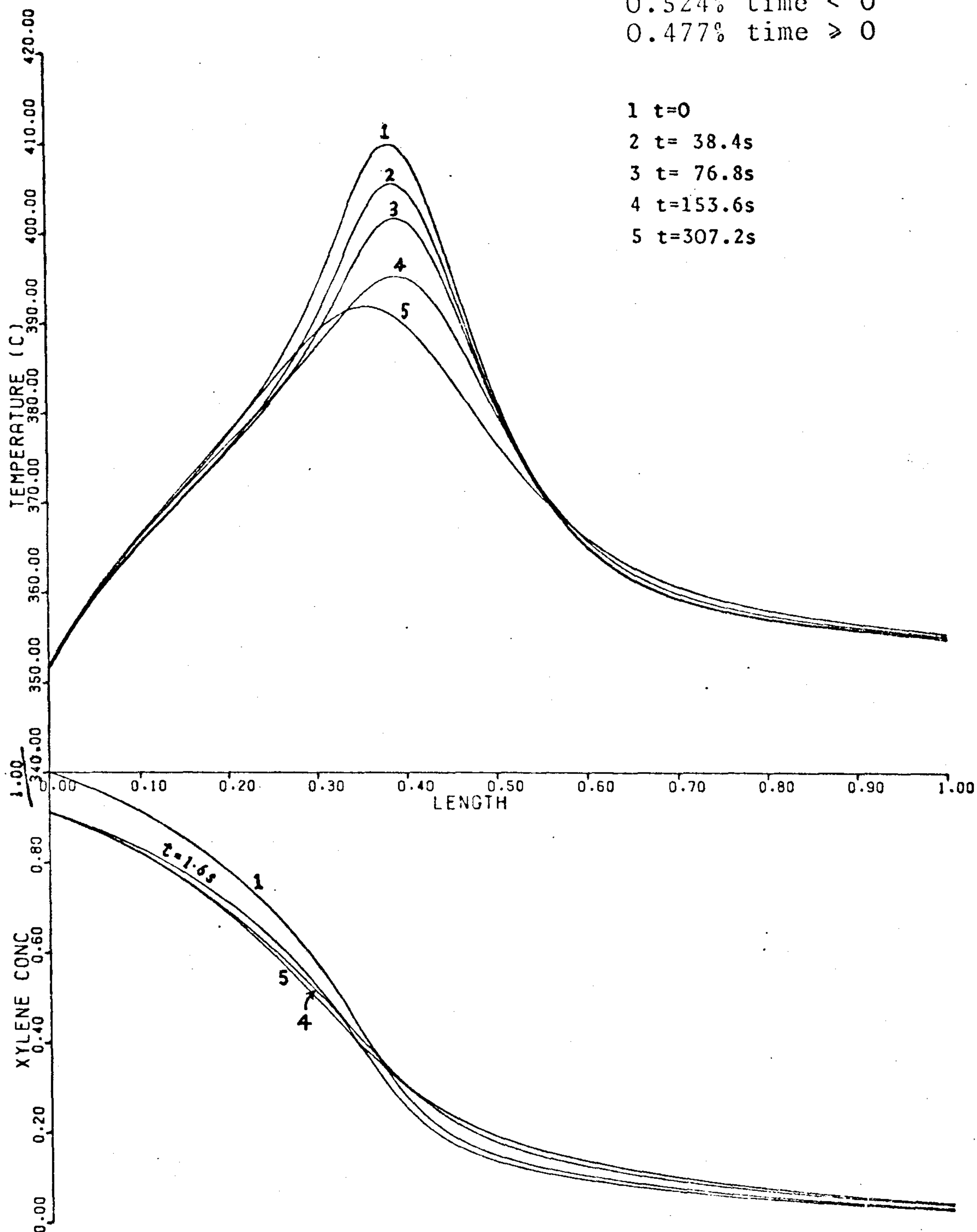
RUN 21A



Graph 4.34. Theoretical and experimental axial temperatures for a xylene concentration step decrease.

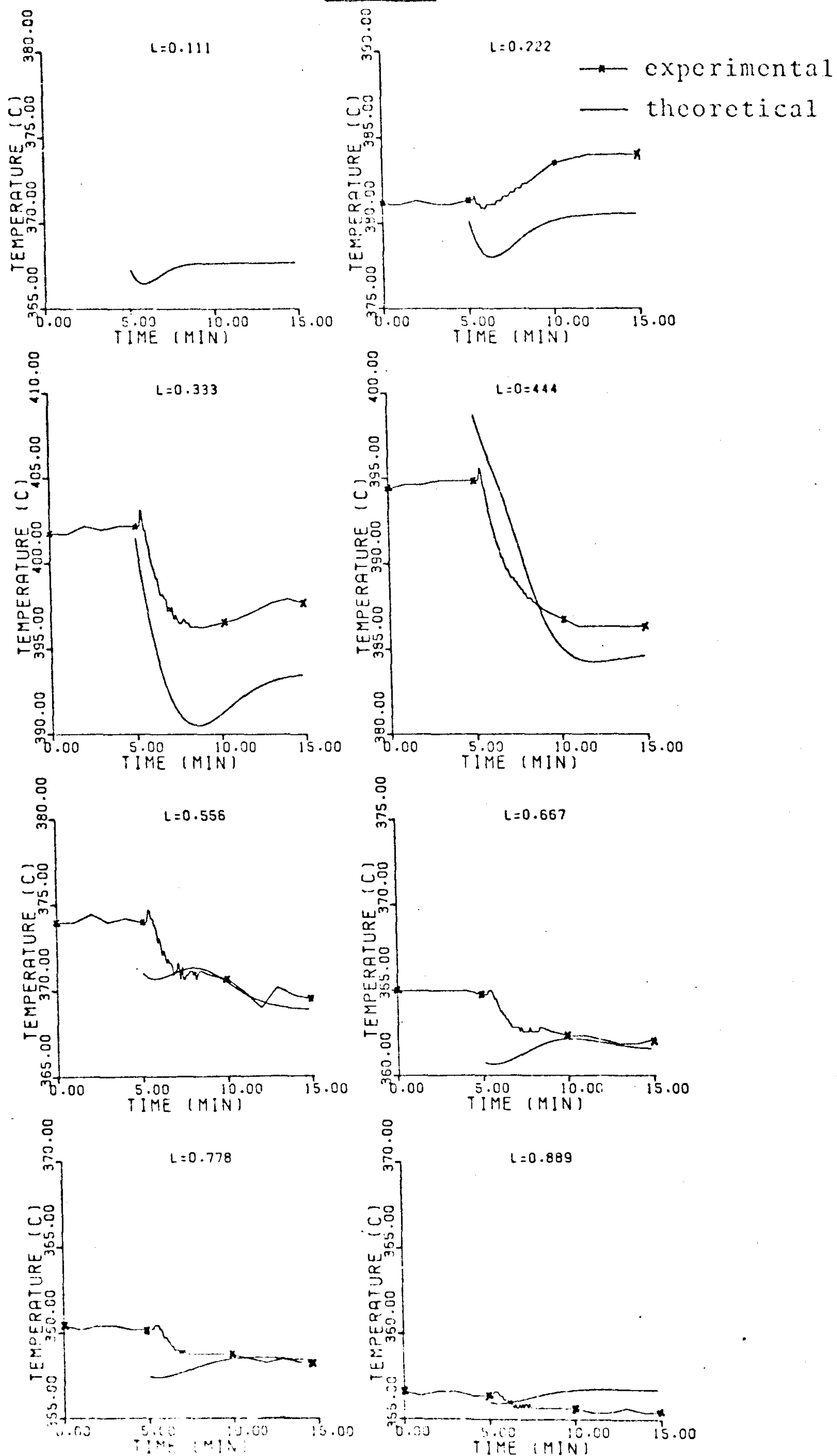
RUN 30A

Gas Flow Rate 477. 1/hr
Inlet Xylene Concentration
0.524% time < 0
0.477% time ≥ 0



Graph 4.35. Theoretical axial temperature and concentration profiles for a xylene concentration step decrease.

RUN 30A

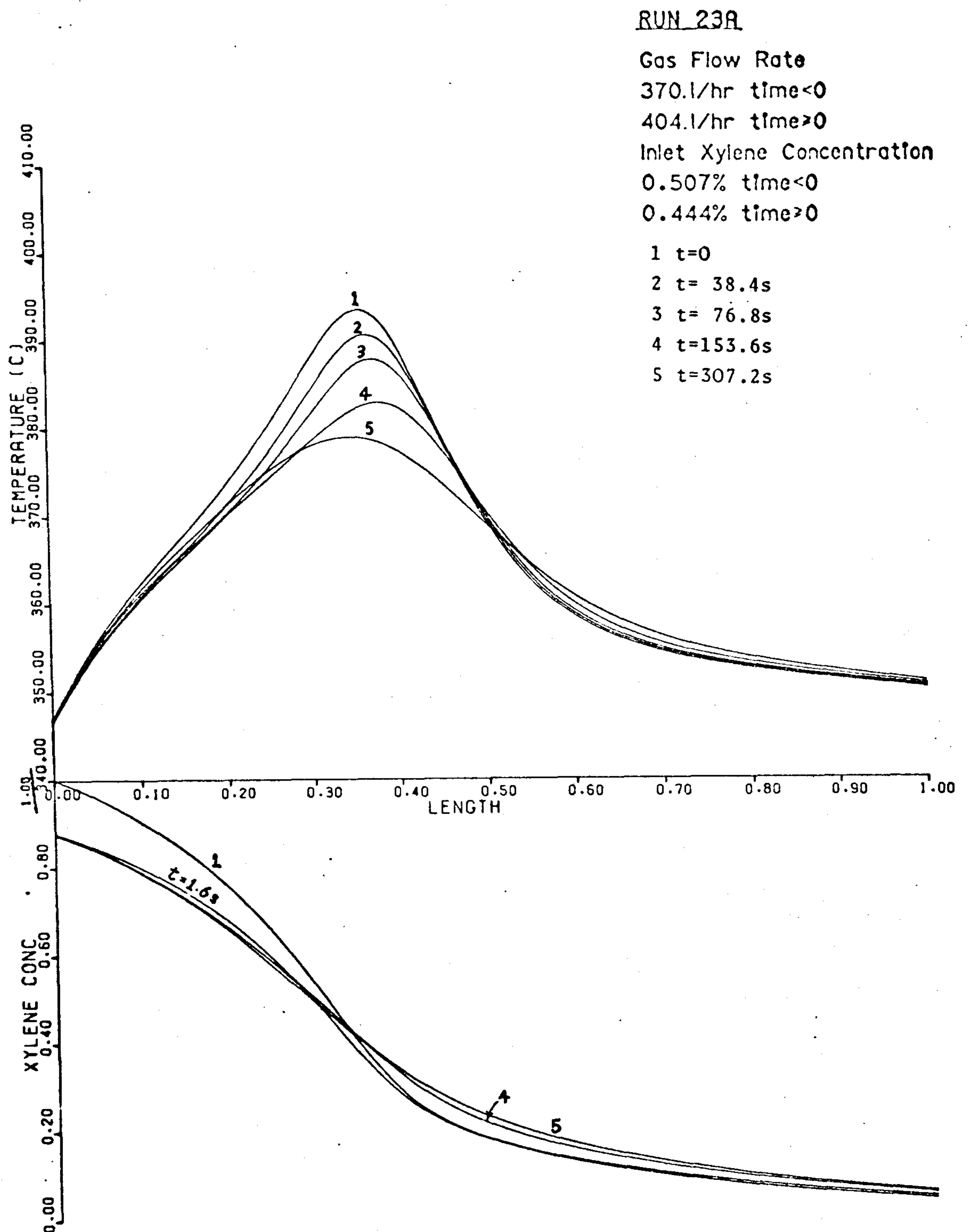


Graph 4.36. Theoretical and experimental axial temperatures for a xylene concentration step decrease.

resulting from the stiffness of the differential equations, up to 4°C in the worst case.

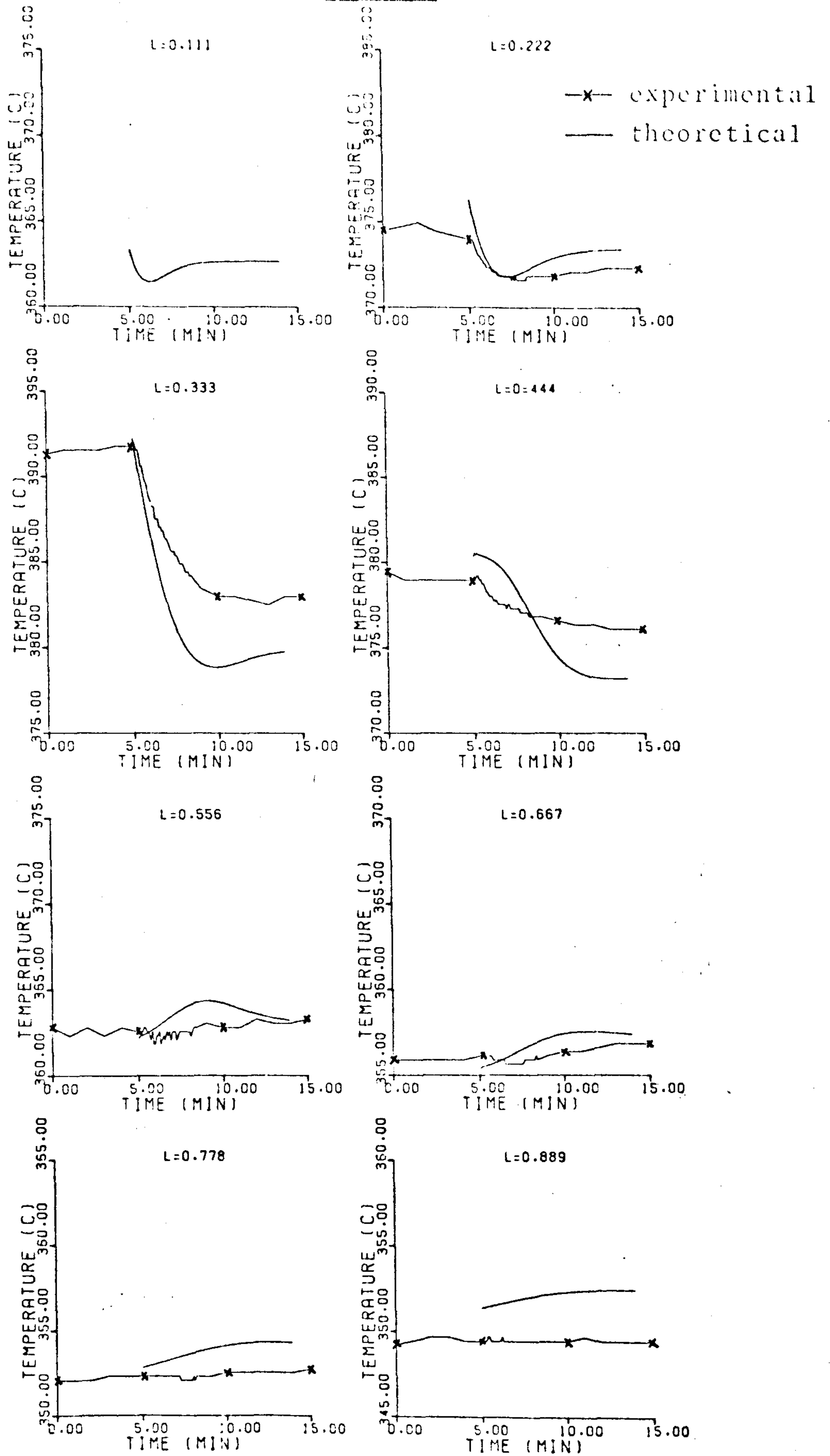
When the air flow rate was decreased, resulting in an increase in the o-xylene flow rate and hence a greater increase in the o-xylene concentration than that which would have been expected (see chapter 3), the temperature at the dimensionless position 0.222 stayed approximately constant. The hot spot moved very slightly towards the inlet and increased in height, see graph 4.17. The anomolous behaviour originally found is not obvious (see graph 4.19), over the first part of the reactor in this case. Due to the decrease in the total gas flow rate, all the heat and mass transfer parameters would decrease, and the slight forward movement of the hot spot would balance the expected temperature decrease of the wrong way behaviour. Again this effect was completely reversible experimentally, see graph 4.16. The model for the flow rate increase (graph 4.37) shows that the hot spot is actually stationary, which is in agreement with the experimental results. Graphs 4.37 to 4.39 of the model, show a small initial overshoot of the final steady state for the first part of the reactor, however the trends are well demonstrated for the latter part of the reactor.

Due to the large amount of computer time necessary to calculate one transient, normally 1700 seconds on a CDC 6400, no non-linear regression of the dynamic parameters was carried out, so that the time constants for the conversion of V_2O_5 to a lower non-active oxidation state, and



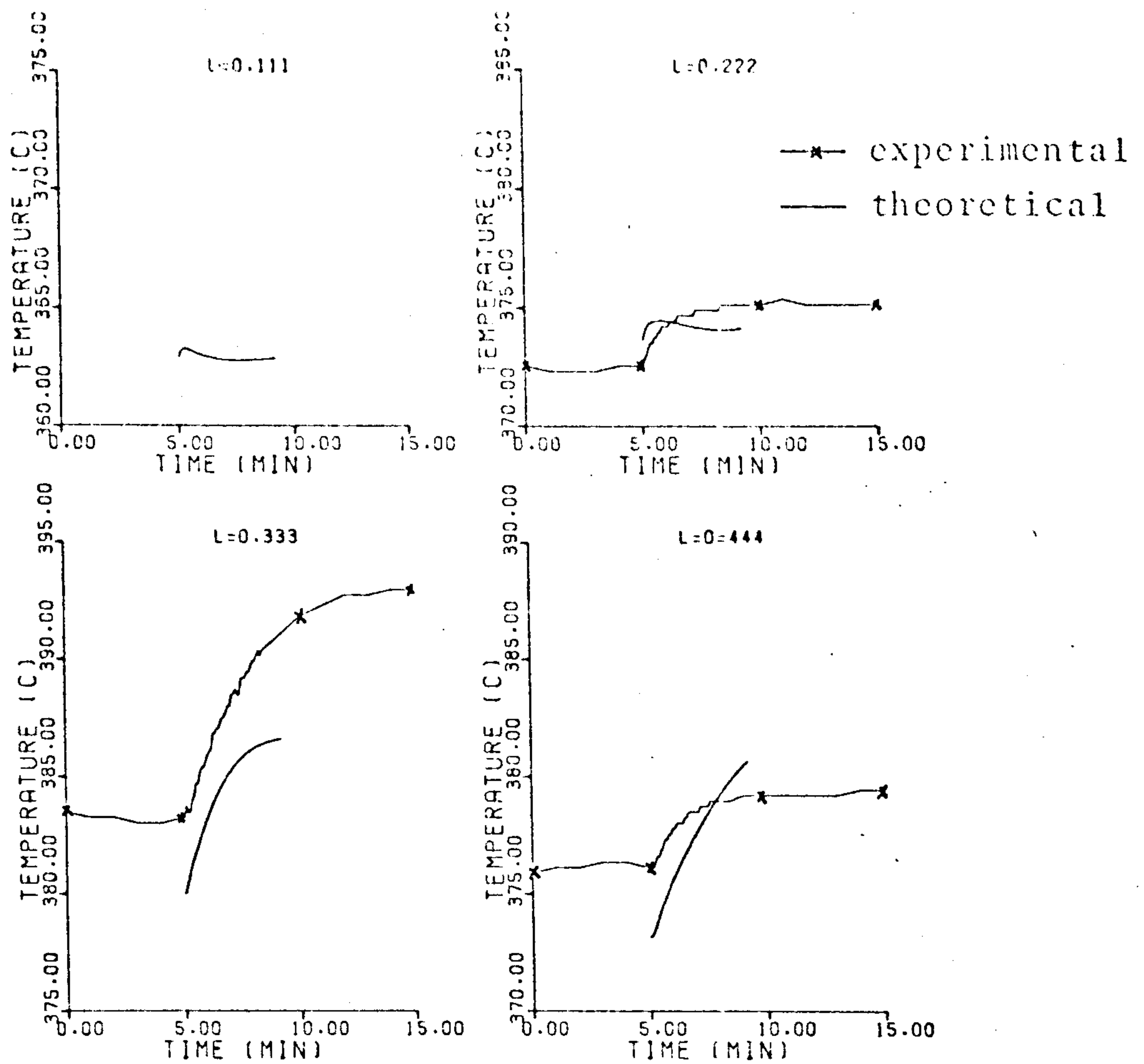
Graph 4.37. Theoretical profiles for a xylene concentration step decrease and a gas rate step increase.

RUN 23A



Graph 4.38. Theoretical and experimental temperatures for a xylene concentration step decrease and a gas rate step increase.

RUN 25B



Graph 4.39. Theoretical and experimental temperatures for a xylene concentration step increase and a gas rate step decrease.

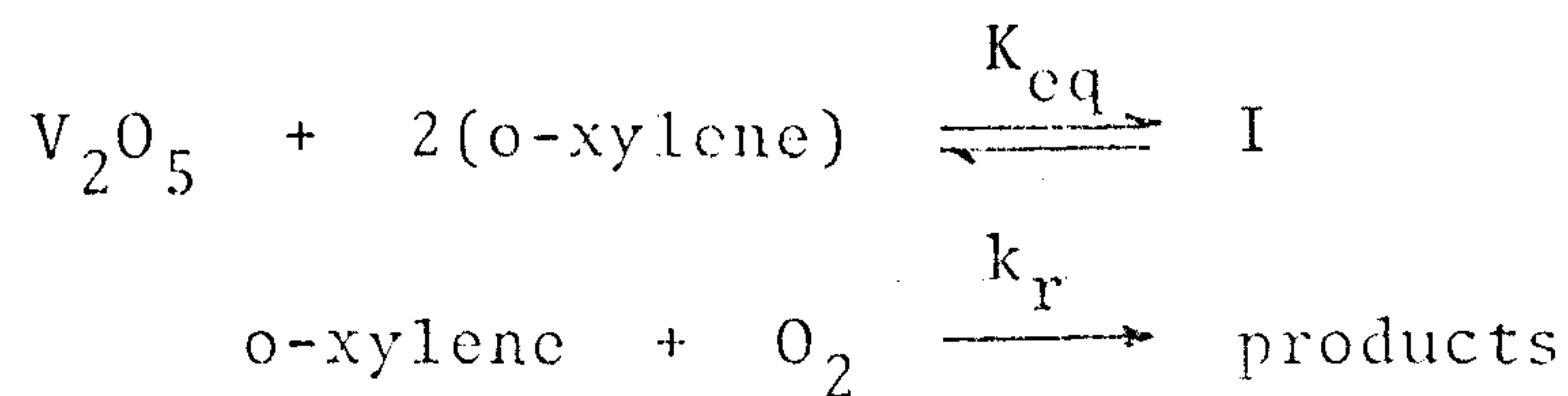
the reverse reaction, were approximately determined by a few trials. The original literature heat capacity of the bed 0.839 KJ/Kg.°C was used unchanged in the dynamic modelling.

The time constant derived from the dynamic modelling, for the deactivation reaction, was estimated to be 10 seconds (rate constant = 0.1 s^{-1}). For higher values of the time constant the overshoot for run 19B, when the concentration was increased from 0.397 to 0.515 mole%, was very large and resulted in a breakdown of the computing algorithm. With this low value of the time constant, poor convergence of the temperature profiles to the final steady state has resulted, due to the stiffness of the partial differential equations.

For the reverse case, a decrease in the outlet o-xylene concentration, a time constant of 10 seconds for the catalyst reactivation reaction results in the disappearance of the initial right way behaviour completely. This is due to the exponential temperature dependence of the rate of oxidation of the o-xylene, so that the overall system is definitely not first order. All the graphs shown for the reactivation of the catalyst have a time constant of 100 seconds. Of these, only run 21A (see graph 4.34) indicates that the time constant is too large. A final value therefore for the catalyst reactivation time constant is approximately 50 seconds (rate constant = 0.02 s^{-1}).

The yield in the pilot plant reactor used for the partial oxidation of o-xylene to phthalic anhydride was found to average 78% or 109 Kg phthalic anhydride per 100 Kg o-xylene with a purity of greater than 97 mole% at a bath temperature of 350 °C. This is comparable to the yield obtained commercially. It was shown that the amount of carbon monoxide produced was not negligible and had to be included in the calculation of the overall heat of reaction.

The axial temperature profiles showed anomolous behaviour for the first quarter of the length of the reactor where an increase in the inlet o-xylene concentration resulted eventually in a decrease to the new steady state temperature, hence there must have been an overall decrease in the heat evolved per unit reactor volume by the reactions taking place. As the possible network of reactions was modelled by a single overall reaction, the rate of this reaction must decrease at high o-xylene concentrations. The physical properties of the system were first eliminated as a possible cause, leaving some kinetic effect where the apparent order of reaction must become negative at high o-xylene concentrations. This eliminates most of the reaction models that have been tried for this or similar systems leaving the bimolecular Langmuir-Hinshelwood and the previously derived catalyst deactivation model. The latter model was selected as the simplest feasible model for both the steady state and dynamic modelling carried out.



As the concentration of o-xylene increases, the active V_2O_5 is deactivated to a lower inactive oxidation state. The overall rate of reaction is proportional to the V_2O_5 concentration resulting in the equation

$$R_r = \frac{k_r C_x}{1 + K_{eq} C_x^2}$$

All the modelling carried out was based on the catalyst deactivation model with an estimated value for the equilibrium constant K_{eq} of 9.00×10^4 . This defines the order of reaction, initially 1.0 at zero o-xylene concentration to be zero at 0.333 mole%. Above this concentration, the order of reaction is negative.

The reaction modelling carried out solving the homogeneous partial differential equations proved to be of the same accuracy as the heterogeneous case using literature values for the heat and mass transfer coefficients between the gas phase and the catalyst pellets. The parameters calculated from the non-linear regression analysis were 1.105×10^8 KJ/Kmole for the activation energy E_a , with an error of $\pm 4\%$, 20.4 for the exponential frequency factor S with an error of $\pm 6\%$. The following correlation is suggested for the wall heat transfer coefficient

$$\text{Nu} = 8.23 + 0.054 \text{ Re Pr}$$

This is almost identical to the correlation proposed by

Yagi and Wakao (72) for the data of Plautz and Johnstone (67). To maintain an accurate fit over all the data, the effective radial conductivity had to be increased, as the inlet o-xylene concentration increased, so that a correlation of the following type is suggested

$$\frac{k_e}{k_g} = \frac{k_e^0}{k_g} + 0.10 \text{ Re Pr}$$

where the stagnant conductivity term k_e^0/k_g increases from 11.7 to 26.0 as the inlet o-xylene concentration increases from 0.31 to 0.6 mole%. The necessity for this is to compensate for either the effect of axial dispersion of heat or excessive temporary deactivation of the catalyst at the higher temperatures encountered with higher inlet o-xylene concentrations. The lowest value for the stagnant conductivity term was just slightly above the literature correlations for non-metallic packed beds. The literature correlations available for the pellet heat and mass transfer correlations are reasonable. At the temperatures studied, up to 410°C, film heat and mass transfer limitations do not occur.

For the modelling of the dynamic case, the trends of the experimental temperature profiles were well demonstrated by estimating the forward reaction for the deactivation of the V_2O_5 to have a time constant of 10 seconds with 50 seconds as the time constant for the catalyst reactivation reaction. The overall wrong way behaviour as well as the small amount of initial right way behaviour of the first part of the reactor were shown. This behaviour could also be demonstrated by the slightly more complex bimolecular

Langmuir-Hinshelwood model.

The orthogonal collocation method proved to be well suited for the solution of the partial differential equations for both the homogeneous and heterogeneous models, and especially for carrying out the non-linear regression analysis. The application of the orthogonal collocation method in all three dimensions for solution of the dynamic case proved to be satisfactory for normal first order reaction models. For the inclusion of the catalyst deactivation effect however, the error and the computing time increased drastically as the time constant for the catalyst deactivation reaction decreased, resulting in a "stiff" set of equations.

At low bath temperature 340-346°C, two hot spots were observed which implies that at least 3 series reactions were taking place. The simplest most favoured model was



In these runs the average phthalic anhydride yield was 65%.

SUGGESTIONS FOR FURTHER WORK

To improve stability of the axial temperature profile, especially at high inlet concentrations of o-xylene, the reactor bath should have some form of forced convection imposed upon it. This could be achieved by using a fluidised bed or a salt bath with mechanical agitation, a circulation pump or injection of air or nitrogen to improve the heat transfer.

Improvement of the analysis and the sampling of the concentration at intermediate points along the bed would result in improved data to model the system as a network of reactions each with its own heat of reaction and not an overall heat of reaction as used in this study. All of these are being incorporated in a continued large scale study.

If possible, heat transfer data should be obtained under non-reactive conditions to produce correlations for the system as the values in the literature are extremely scattered. An improvement may be obtained in the non-linear regression for the effective radial conductivity and the wall heat transfer coefficient, from either separate analysis or with reaction if the correlation between these two parameters is eliminated by using the variables U and either h_w or k_e as defined by the equation

$$\frac{1}{U} = \frac{1}{h_w} + \frac{R}{1.91 k_e}$$

or an equation of similar form.

A study should be undertaken to determine if a distinction can be made between the catalyst deactivation model and the bi-molecular Langmuir-Hinshelwood model, especially under dynamic conditions. To solve the partial differential equations accurately however, both these cases may require the use of a different algorithm to eliminate the stiffness in the energy equation. This is due to the large difference in the time constants between the reactor temperature and the kinetic constant either for catalyst deactivation or adsorption/desorption of the reactants.

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Appendix I

MATHEMATICAL MODELS

1. Homogeneous Steady State

Energy balance

$$C_{Pg} \rho_g u \frac{\partial \theta}{\partial z'} = - R_r \Delta H_r + k_e \frac{1}{r'} \frac{\partial}{\partial r'} (r' \frac{\partial \theta}{\partial r'}) \quad (I.1)$$

with the boundary conditions

$$\begin{aligned} k_e \frac{\partial \theta}{\partial r'} &= - h_w (\theta - \theta_c) & \text{at } r' = R \\ \theta &= \theta_o & \text{at } z' = 0 \end{aligned}$$

Mass balance

$$u \frac{\partial C'}{\partial z'} = - R_r + \epsilon D_e \frac{1}{r'} \frac{\partial}{\partial r'} (r' \frac{\partial C'}{\partial r'}) \quad (I.2)$$

with the boundary conditions

$$\begin{aligned} \frac{\partial C'}{\partial r'} &= 0 & \text{at } r' = R \\ C' &= C_o & \text{at } z' = 0 \end{aligned}$$

Dimensionless transformations

$$\frac{\partial T}{\partial z} = \beta g(T, C) + \alpha \frac{1}{r} \frac{\partial}{\partial r} (r \frac{\partial T}{\partial r}) \quad (I.3)$$

$$\frac{\partial C}{\partial z} = - \frac{g(T, C)}{C_o} + \gamma \frac{1}{r} \frac{\partial}{\partial r} (r \frac{\partial C}{\partial r}) \quad (I.4)$$

with the boundary conditions

$$\begin{aligned} \frac{\partial T}{\partial r} &= - Bi (T - T_c) & \text{at } r = 1 \\ \frac{\partial C}{\partial r} &= 0 & \text{at } r = 1 \\ T &= C = 1 & \text{at } z = 0 \end{aligned}$$

where

$$\begin{aligned} T &= \frac{\theta - \theta_{base}}{\theta_o - \theta_{base}} & C &= \frac{C'}{C_o} \\ r &= \frac{r'}{R} & z &= \frac{z'}{Z} \\ \beta &= \frac{-\Delta H_r}{C_{Pg}(\theta_o - \theta_{base})} & \alpha &= \frac{k_e Z}{C_{Pg} GR^2} \end{aligned} \quad (I.5)$$

$$g(T, C) = \frac{R_r Z}{G} \quad \gamma = \frac{\epsilon D_c Z}{R^2 u} \quad (I.6)$$

$$Bi = \frac{h_w R}{k_e}$$

2. Heterogeneous Steady State

Energy balance

$$- \Delta H_r R_r = h_p (\theta_p - \theta_b) a - k_{ep} \frac{1}{r'} \frac{\partial}{\partial r'} (r' \frac{\partial \theta_p}{\partial r'}) \quad (I.7)$$

$$C_{Pg} \rho_g u \frac{\partial \theta_b}{\partial z'} = h_p (\theta_p - \theta_b) a + k_{eb} \frac{1}{r'} \frac{\partial}{\partial r'} (r' \frac{\partial \theta_b}{\partial r'}) \quad (I.8)$$

with the boundary conditions

$$k_{ep} \frac{\partial \theta_p}{\partial r'} = - h_{wp} (\theta_p - \theta_c) \quad \text{at } r' = R$$

$$k_{eb} \frac{\partial \theta_b}{\partial r'} = - h_{wb} (\theta_b - \theta_c) \quad \text{at } r' = R$$

$$\theta_b = \theta_o \quad \text{at } z' = 0$$

As the solid radial conductivity k_{ep} is to be lumped in an overall gas phase conductivity, the last term in equation (I.7) can be ignored. Similarly the pellet to wall heat transfer is lumped in the following overall gas phase to wall heat transfer boundary condition.

$$k_e \frac{\partial \theta_b}{\partial r'} = - h_w (\theta_b - \theta_c) \quad \text{at } r' = R$$

Mass balance

$$- R_r = K_G (C'_p - C'_b) a \quad (I.9)$$

$$u \frac{\partial C'_b}{\partial z'} = K_G (C'_p - C'_b) a + \epsilon D_e \frac{1}{r'} \frac{\partial}{\partial r'} (r' \frac{\partial C'_b}{\partial r'}) \quad (I.10)$$

with the boundary conditions

$$\begin{aligned}\frac{\partial C_b'}{\partial r'} &= 0 & \text{at } r' = R \\ C_b' &= C_o' & \text{at } z' = 0\end{aligned}$$

Dimensionless transformations

Energy Balance

$$\beta g(T_p, C_p) = St_{ht}(T_p - T_b) \quad (I.11)$$

$$\frac{\partial T_b}{\partial z} = St_{ht}(T_p - T_b) + \alpha \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_b}{\partial r} \right) \quad (I.12)$$

Mass Balance

$$- \frac{g(T_p, C_p)}{C_o} = St_{mt}(C_p - C_b) \quad (I.13)$$

$$\frac{\partial C_b}{\partial z} = St_{mt}(C_p - C_b) + \gamma \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_b}{\partial r} \right) \quad (I.14)$$

with boundary conditions

$$\frac{\partial T_b}{\partial r} = -Bi(T_b - T_c) \quad \text{at } r = 1$$

$$\frac{\partial C_b}{\partial r} = 0 \quad \text{at } r = 1$$

$$T_b = C_b = 1 \quad \text{at } z = 1$$

The modified Stanton numbers for heat and mass transfer are defined as:

$$St_{ht} = \frac{h_p}{C_{p_g} G} a Z \quad St_{mt} = \frac{K_G}{u} a Z$$

3. Dynamic Heterogeneous Model

Energy balance

$$- \Delta H_r R_r = h_p(\theta_p - \theta_b) a + C_{p_p} \rho_p \frac{\partial \theta_p}{\partial t} \quad (I.15)$$

$$C_{p_g} \rho_g u \frac{\partial \theta_b}{\partial z} = h_p(\theta_p - \theta_b) a + k_e \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \theta_b}{\partial r} \right) - \epsilon C_{p_g} \rho_g \frac{\partial \theta_b}{\partial t} \quad (I.16)$$

with boundary conditions as equation (I.8)

Mass balance

$$- R_r = K_G(C'_p - C'_b) a + a \delta \frac{\partial C'_p}{\partial t} \quad (I.17)$$

$$u \frac{\partial C'_b}{\partial z} = K_G(C'_p - C'_b) a + \epsilon D_e \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C'_b}{\partial r} \right) - \epsilon \frac{\partial C'_b}{\partial t} \quad (I.18)$$

with boundary conditions as for equation (I.10), and the temperature and concentration profiles defined at time $t=0$.

As the heat capacity of the gas is negligible compared with that of the catalyst, the last term of equation (I.16) can be ignored. The volume of the boundary layer is negligible therefore the last term in equation (I.17) can be ignored.

Dimensionless transformations

Energy balance

$$\beta g(T_p, C_p) = St_{ht}(T_p - T_b) + \xi \frac{\partial T_p}{\partial t} \quad (I.19)$$

$$\frac{\partial T_b}{\partial z} = St_{ht}(T_p - T_b) + \alpha \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_b}{\partial r} \right) \quad (I.20)$$

Mass balance

$$- \frac{g(T_p, C_p)}{C_o} = St_{mt}(C_p - C_b) \quad (I.21)$$

$$\frac{\partial C_b}{\partial z} = St_{mt}(C_p - C_b) + \gamma \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_b}{\partial r} \right) - \epsilon \frac{\partial C_b}{\partial t} \quad (I.22)$$

with boundary conditions as for equations (I.12) and (I.14) and the temperature and concentration profiles defined at time $t=0$.

where

$$\xi = \frac{C_{p_p} \rho_p}{C_{p_g} \rho_g} \frac{z}{t_r u} \quad t_r = \epsilon \frac{z}{u}$$

Appendix II THE ORTHOGONAL COLLOCATION METHOD

Introduction

The orthogonal collocation method is one of a general class of approximate methods known as the method of weighted residuals (104,105), which includes the Galerkin integral, and moments methods as special cases. In these methods the unknown solution of a system of differential equations, with boundary and initial conditions, is expanded in a trial series whose functional dependance on position is chosen, but which includes undetermined functions of time, or a further dimension. These functions are found by requiring that the trial solution approximates the differential equation, according to various criteria.

Derivation Of The Orthogonal Collocation Method

For Radial Profiles

As a specific example solve the dimensionless equation (I.3).

$$-\frac{\partial T}{\partial z} + \beta g(T,C) + \alpha \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) = 0 \quad (\text{II.1})$$

where

$$\frac{\partial T}{\partial r} = -Bi(T - T_c) \quad \text{at } r = 1 \quad (\text{II.1a})$$

$$T = 1 \quad \text{at } z = 0$$

The temperature and concentration are expanded in a series $\sum a_i(z)P_i(r)$ of defined functions of radius, $P_i(r)$, multiplied by unknown functions of z , $a_i(z)$. As the solution for the radial case must be symmetrical about $r = 0$ expand the trial function $T(z,r)$ in terms of r^2 . Therefore define the trial solution for a fixed radial

section as

$$T_N(z, r) = \sum_{i=0}^N a_i(z) P_i(r^2) \quad (II.2)$$

This trial function is substituted into the partial differential equation (II.1) to form the residual.

$$R(a_i, z, r) = - \frac{\partial T}{\partial z} + \beta g(T, C) + \alpha \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \sum_{i=0}^N a_i(z) P_i(r^2) \right) \quad (II.3)$$

If the trial function were the exact the solution, the residual would be zero. In the various methods of weighted residuals, the constants $a_i(z)$ are derived in such a way that the residual is forced to be zero in some average sense. Therefore set the weighted integral of the residual, $\int_r w_j R(a_i, z, r) dr$ to zero, with the weighting function still to be selected.

Taking the weighted integral of equation (II.3)

$$0 = \int_r w_j \left(- \frac{\partial T}{\partial z} + \beta g(T, C) \right) dr + \alpha \sum_{i=1}^N a_i(z) \int_r w_j \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} P_i(r^2) \right) dr \quad (II.4)$$

In the collocation method, the weighting functions are chosen to be the displaced Dirac delta function

$$w_j = \delta(r - r_j)$$

which has the properties

$$\int_r w_j U dr = U|_{r_j}$$

$$\int_r w_j \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} P_i(r^2) \right) dr = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} P_i(r^2) \right) |_{r_j}$$

So that this weighting function forces the solution to be exact at the specified points r_j , the collocation points.

Therefore equation (II.4) reduces to

$$0 = - \left. \frac{\partial T}{\partial z} \right|_{r_j} + \beta \left. g(T, C) \right|_{r_j} + \alpha \sum_{i=1}^N D_{ji} a_i(z) \quad (\text{II.5})$$

where

$$D_{ji} = \left. \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} P_i(r^2) \right) \right|_{r_j} \quad (\text{II.6})$$

and

$$i = 1, 2, \dots, N$$

$$j = 1, 2, \dots, (N-1)$$

i.e. this is not valid at the boundary.

If the boundary condition is of the type $T=1$ at $r=1$ then it is included in the trial function by specifying the $a_i(z)$ in equation (II.2) so that the trial function fits the boundary conditions and equations (II.5) and (II.6) are now valid at the boundary. The boundary condition in this case however is

$$0 = \frac{\partial T}{\partial r} + Bi (T - T_c) \quad \text{at } r = 1 \quad (\text{II.7})$$

Following the same steps as previously

$$0 = Bi (T - T_c) \big|_{r=1} + \sum_{i=1}^N C_{ji} a_i(z) \quad (\text{II.8})$$

where

$$C_{ji} = \frac{d}{dr} P_i(r^2) \quad (\text{II.9})$$

and

$$i = 1, 2, \dots, N$$

$$j = N \text{ only.}$$

For problems involving chemical reactions with an Arrhenius temperature dependence, the degenerate orthogonal collocation method is the most feasible, as the other

methods of weighted residuals normally require evaluation of complicated integrals involving exponential functions.

In the collocation method, the differential equation is satisfied only at discrete points, called collocation points. Originally the choice of both the trial function and the collocation points for boundary value problems was somewhat arbitrary until Villadsen and Stewart (44) defined the trial functions as orthogonal polynomials and the collocation points as the roots of these equations. The collocation points are also the optimal quadrature points for the numerical integration of the solution over the same region. The orthogonal polynomials are defined by:

$$\int_0^1 W(r^2) P_i(r^2) P_j(r^2) r^{\alpha-1} dr = 0$$

where $j = 1, 2, \dots, (i-1)$

$W(r^2)$ is the weighting factor

$P_i(r^2)$ is a polynomial in r^2 of degree i

α the geometric factor = 1 for planar geometry

= 2 for cylindrical geometry

= 3 for spherical geometry

The weighting function $W(r^2)=1$ gives rise to the Legendre polynomials. P_0 is taken as 1 therefore this completely defines the trial functions

$$P_1 = 1 - 2r^2 \quad P_2 = 1 - 6r^2 + 6r^4 \quad P_3 = \dots$$

whereas $W(r^2)=1-r^2$ defines the Jacobi polynomials

$$P_0 = 1 \quad P_1 = 1 - 3r^2 \quad P_2 = 1 - 8r^2 + 10r^4 \quad \dots$$

The collocation points are denoted by r_j and are the roots

of the orthogonal polynomial

$$P_N(r^2) = 0 \quad j = 1, 2, \dots, N$$

Since the functions P_i are known, C_{ji} and D_{ji} can be calculated from equations (II.6) and (II.9) respectively. Therefore equation (II.5) for collocation points $\leq N-1$ and equation (II.8) for the N th. collocation point at the boundary can be solved simultaneously by an iterative method to find the $a_i(z)$ which leads to the approximate solution in equation (II.2).

Computer programmes however are simpler if written in terms of the solution at the collocation points r_j rather than trying to evaluate the $a_i(z)$ and the trial function. As $P_N(r^2)$ is a polynomial of degree N in r^2 equation (II.2) can be written as

$$T(z, r) = \sum_{i=1}^{N+1} r^{2i-2} d_i \quad (II.10)$$

or evaluating at the collocation points

$$T(z, r_j) = \sum_{i=1}^{N+1} r_j^{2i-2} d_i \quad (II.11)$$

Taking the first derivative and the Laplacian of this expression

$$\left. \frac{\partial}{\partial r} T(z, r_j) \right|_{r_j} = \sum_{i=1}^{N+1} \left. \frac{d}{dr} r^{2i-2} \right|_{r_j} d_i \quad (II.12)$$

$$\left. \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} T(z, r_j) \right) \right|_{r_j} = \sum_{i=1}^{N+1} \frac{1}{r} \left. \frac{d}{dr} \left(r \frac{d}{dr} r^{2i-2} \right) \right|_{r_j} d_i \quad (II.13)$$

These equations can be rewritten in matrix notation as follows. Note that the $(N+1)$ th. collocation point is $r=1$ and square matrices have $(N+1)^2$ elements.

$$T = Qd \quad \frac{\partial T}{\partial r} = Cd \quad \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) = Dd \quad (\text{II.14})$$

where:

$$Q_{ji} = r_j^{2i-2} \quad C_{ji} = \left. \frac{d}{dr} r^{2i-2} \right|_{r_j} \quad D_{ji} = \left. \frac{1}{r} \frac{d}{dr} \left(r \frac{d}{dr} r^{2i-2} \right) \right|_{r_j} \quad (\text{II.15a,b,c})$$

Solving for d

$$\frac{\partial T}{\partial r} = CQ^{-1}T = AT \quad (\text{II.16})$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) = DQ^{-1}T = BT \quad (\text{II.17})$$

Therefore the derivatives are expressed in terms of the values of the function at the collocation points. By substituting equations (II.16) and (II.17) in equation (II.1) and (II.1a) the original partial differential equation is now reduced to an easily solvable ordinary differential equation.

$$- \left. \frac{dT}{dz} \right|_{r_j} + \beta g(T,C) \big|_{r_j} + \alpha \sum_{i=1}^{N+1} B_{ji} T_i = 0 \quad (\text{II.18})$$

with the boundary condition

$$- \sum_{i=1}^{N+1} A_{N+1,i} T_i = B_i (T_{N+1} - T_w) \text{ at } r = 1 \quad (\text{II.18a})$$

For a first approximation, the simplest case $N=1$ has only one internal radial collocation point. If Jacobi polynomials are used the collocation point $r_1=1/\sqrt{3}$. From appendix IV substitute the values for matrices A and B into equations (II.18) and (II.18a).

$$\frac{dT_1}{dz} = \beta g(T,C)_1 + \alpha \begin{bmatrix} -6 & 6 \end{bmatrix} \begin{bmatrix} T_1 \\ T_{N+1} \end{bmatrix} \quad (\text{II.19})$$

$$- \begin{bmatrix} 3 & 3 \end{bmatrix} \begin{bmatrix} T_1 \\ T_{N+1} \end{bmatrix} = Bi \begin{bmatrix} T_{N+1} - T_w \end{bmatrix} \quad (II.19a)$$

Combining equations (II.19) and (II.19a)

$$\frac{dT_1}{dz} = \left(\frac{6\alpha Bi}{Bi + 3} \right) (T_w - T_1) + \beta g(T, C)_1 \quad (II.20)$$

Equation (II.20) is very similar to the one-dimensional lumped parameter model

$$\frac{dT}{dz} = - Nu' (T - T_w) + \beta g(T, C) \quad (II.21)$$

where

$$Nu' = \frac{2UZ}{C_{p_g} GR}$$

and U = lumped heat transfer coefficient.

The lumped parameter model assumes a constant temperature across the reactor. As the simple orthogonal collocation case considered has only one internal collocation point, equation (II.20) refers to a temperature at a particular radius where the temperature varies parabolically with r .

Equating $6\alpha Bi/(Bi+3)$ from equation (II.20) to the modified Nusselt number in equation (II.21) and expressing in terms of heat transfer resistances

$$\frac{1}{U} = \frac{1}{h_w} + \frac{R}{3 k_e} \quad (II.22)$$

for Jacobi weighting and similarly for Legendre weighting

$$\frac{1}{U} = \frac{1}{h_w} + \frac{R}{4 k_e} \quad (II.23)$$

These equations are of the same form as the expressions for the lumped heat transfer coefficient derived theoretically by Beck and Singer (101), and Crider and Foss (102). As Legendre polynomials have a weighting of unity the

rate of reaction is evaluated at the average radial temperature. By using Jacobi polynomials, the reaction rate expression is evaluated at a temperature above the average radial temperature. In low order collocation solutions, this approximates more closely the average rate of reaction due to the exponential effect of the temperature where the average temperature does not yield the average rate of reaction. With higher order solutions, the difference between weighting methods becomes negligible.

Derivation of the Orthogonal Collocation Method For Axial Profiles

As the solution for the axial case will not be symmetric in the region $0 \leq z \leq 1$ expand the trial function in terms of z

$$T_M(z,r) = \sum_{i=0}^{M+1} a_i(r) P_i(z) \quad (II.24)$$

substituting the boundary condition at the inlet

$$T_M(z,r) = T(0,r) + \sum_{i=0}^{M+1} a_i(r) P_i(z) \quad (II.25)$$

with the orthogonality requirement

$$\int_0^1 W(z) P_i(z) P_j(z) dz = 0$$

Unlike the previous section there is no general rule for choosing the weighting factor $W(z)$, therefore select the simplest case i.e. the Legendre polynomials.

$$\begin{aligned} W(z) &= 1 & P_0 &= 1 & P_1 &= 1 - 2z \\ & & P_2 &= 1 - 6z + 6z^2 & P_3 &= \dots \end{aligned}$$

To simplify the computer solution as before solve equation (II.25) in terms of the solution at the collocation points.

$$T(z,r) = \sum_{i=1}^{M+2} z^{i-1} d_i \quad (II.26)$$

Included in the summation term is $T(0,r)$ of equation (II.25) as this is normally equal to 0 or 1. Evaluating equation (II.26) at the collocation points

$$T(z_j,r) = \sum_{i=1}^{M+2} z_j^{i-1} d_i \quad (II.27)$$

Taking the derivative and Laplacian of this expression

$$\frac{\partial}{\partial z} T(z_j,r) \Big|_{z_j} = \sum_{i=1}^{M+2} \frac{d}{dz} z^{i-1} \Big|_{z_j} d_i \quad (II.28)$$

$$\frac{\partial^2}{\partial z^2} T(z_j,r) \Big|_{z_j} = \sum_{i=1}^{M+2} \frac{d^2}{dz^2} z^{i-1} \Big|_{z_j} d_i \quad (II.29)$$

Note that the first collocation point is at $z=0$, the $(M+2)$ th. collocation point is at $z=1$ and that each square matrix has $(M+2)^2$ elements.

$$T = Q*d \quad \frac{\partial T}{\partial z} = C*d \quad \frac{\partial^2 T}{\partial z^2} = D*d \quad (II.30a,b,c)$$

where

$$\begin{aligned} Q_{ji}^* &= z_j^{i-1} & C_{ji}^* &= \frac{d}{dz} z^{i-1} \Big|_{z_j} \\ D_{ji}^* &= \frac{d^2}{dz^2} z^{i-1} \Big|_{z_j} \end{aligned} \quad (II.31a,b,c)$$

Solving for d as before

$$\frac{\partial T}{\partial z} = C*Q^{*-1}T = ET \quad (II.32)$$

$$\frac{\partial^2 T}{\partial z^2} = D*Q^{*-1}T = FT \quad (II.33)$$

The derivatives are now expressed in terms of the values of the function at the collocation points.

Interpolation

To determine the solution, at a point other than a collocation point, equation (II.10) and equation (II.26) are used for interpolating in the radial and axial directions respectively. The interpolation is of order $2N$ radially and $M+1$ axially. For radial interpolation, use equation (II.10)

$$T(z,r) = \sum_{i=1}^{N+1} r^{2i-2} d_i \quad (II.10)$$

where $d = Q^{-1}T$

For centre line conditions expand equation (II.10)

$$T(z,0) = r^0 d_1 + \sum_{i=2}^{N+1} r^{2i-2} d_i$$

$$\text{As } r=0 \quad T(z,0) = d_1 \quad (II.34)$$

where

$$d_1 = \sum_{j=1}^{N+1} (Q^{-1})_{1j} T_j$$

For axial interpolation use equation (II.26) where $d = Q^{-1}T$

Matrices A, B, E and F are listed in appendix IV and Finlayson (105) and Villadsen(106) for low order collocation solutions. For higher order solutions the collocation points are listed in Stroud and Secrest (107). When the collocation points are known Q, C, D and Q*, C*, D* can be calculated from equations (II.15a,b,c) and (II.31a,b,c) respectively. Then A, B, E and F can be calculated from equations (II.16), (II.17), (II,32) and (II.33) respectively.

Convergence

Rigorous proofs of convergence for the orthogonal collocation method have only been obtained for extremely simple problems. Finlayson (108), proves the convergence of the Galerkin method for the solution of radial diffusion and reaction in a tubular packed bed reactor with an Arrhenius type rate of reaction and postulates (105) that if the Galerkin method converges then the collocation method converges. Villadsen and Stewart (44) show that for linear differential equations with constant coefficients that the orthogonal collocation and Galerkin methods yield identical results and that the methods are exact for any even polynomials of degree $< 2N$ where $N+1$ is the total number of collocation points.

Evaluation of Integrals

To evaluate integrals accurately the quadrature formula is used.

$$\int_0^1 f(x^2) x^{a-1} dx = \sum_{j=1}^{N+1} w_j f(x_j^2)$$

To determine the vector w integrate $f(x^2) = x^{2i-2}$

$$\int_0^1 x^{2i-2} x^{a-1} dx = \frac{1}{2i - 2 + a}$$

therefore

$$\sum_{j=1}^{N+1} w_j x_j^{2i-2} = \frac{1}{2i - 2 + a} = f_i$$

as $Q_{ji} = x_j^{2i-2}$

$$wQ = f$$

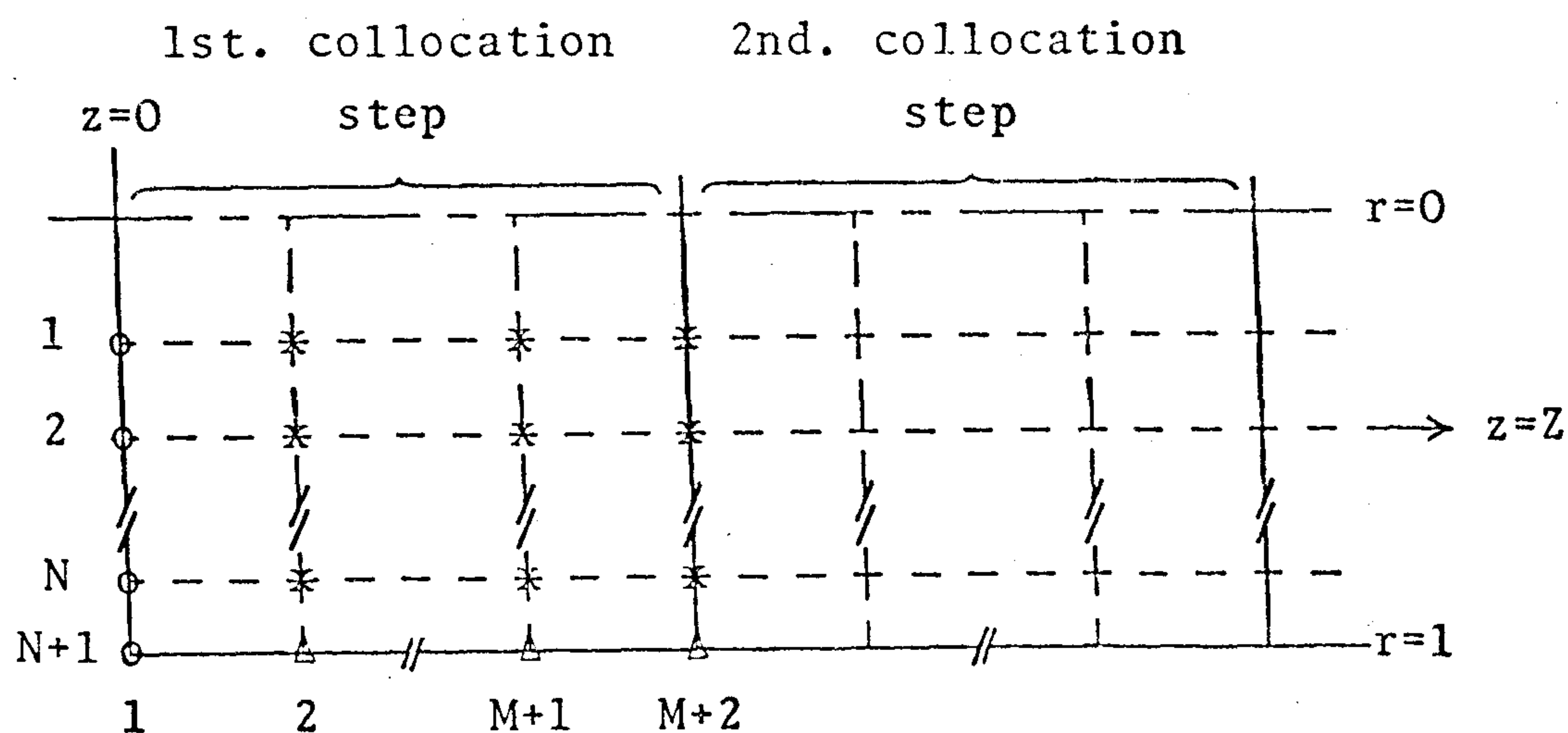
and $w = fQ^{-1}$

Appendix III APPLICATION OF THE ORTHOGONAL COLLOCATION METHOD

METHOD

To solve the relevant partial differential equations by the orthogonal collocation method, the reactor is divided into L equal axial collocation steps, with each step having $N+1$ radial and $M+2$ axial collocation points, see fig III.1. The axial subdivision of the reactor is necessary to improve accuracy while keeping the resulting matrices to a manageable size. As each axial collocation step is a reactor with length Z/L , any terms that include Z , after the dimensionless transformations, must be divided by L so that equations (1.5) and (1.6) have to be modified to

$$\alpha = \frac{k_e}{C_{p_g} G R^2} \frac{Z}{L} \quad \gamma = \frac{D_e}{R^2 u} \frac{Z}{L}$$



- o known temperature and concentration
- x unknown temperature and concentration
- Δ unknown boundary temperature and concentration

Fig III.1 PLAN OF ORTHOGONAL COLLOCATION POINTS

For the general case using Jacobi polynomials with $N=2$ and $M=1$, the radial collocation points are $\sqrt{(4-\sqrt{6})/10}$, $\sqrt{(4+\sqrt{6})/10}$, 1 while the axial collocation points are 0, $\frac{1}{2}$, 1.

For the solution at the internal collocation points, equations (II.17) and (II.32) for the collocation forms of the derivatives, are substituted into equation (I.1) with α modified as above. Similarly for the external collocation points or boundary conditions, as in the simple case $N=1$, demonstrated by equations (II.19) and (II.19a).

$$\begin{bmatrix} T_{11} & T_{21} & T_{31} \\ T_{12} & T_{22} & T_{32} \end{bmatrix} \begin{bmatrix} E_{21} & E_{31} \\ E_{22} & E_{32} \\ E_{23} & E_{33} \end{bmatrix} = \beta \begin{bmatrix} g(T,C)_{21} & g(T,C)_{31} \\ g(T,C)_{22} & g(T,C)_{32} \end{bmatrix} + \alpha \begin{bmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \end{bmatrix} \begin{bmatrix} T_{21} & T_{31} \\ T_{22} & T_{32} \\ T_{23} & T_{33} \end{bmatrix} \quad (\text{III.1})$$

with the boundary conditions

$$\begin{bmatrix} A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} T_{21} & T_{31} \\ T_{22} & T_{32} \\ T_{23} & T_{33} \end{bmatrix} = -Bi \begin{bmatrix} (T_{23}-T_c) & (T_{33}-T_c) \end{bmatrix} \quad (\text{III.1a})$$

with the notation for T_{jk} , C_{jk} , and $g(T,C)_{jk}$ only

j = axial collocation position

k = radial collocation position.

Similarly for the mass balance equations

$$\begin{bmatrix} C_{11} & C_{21} & C_{31} \\ C_{12} & C_{22} & C_{32} \end{bmatrix} \begin{bmatrix} E_{21} & E_{31} \\ E_{22} & E_{32} \\ E_{23} & E_{33} \end{bmatrix} = -\frac{1}{C_o} \begin{bmatrix} g(T,C)_{21} & g(T,C)_{31} \\ g(T,C)_{22} & g(T,C)_{32} \end{bmatrix} + \gamma \begin{bmatrix} B_{11} & B_{12} & B_{13} \\ E_{21} & B_{22} & B_{23} \end{bmatrix} \begin{bmatrix} C_{21} & C_{31} \\ C_{22} & C_{32} \\ C_{23} & C_{33} \end{bmatrix} \quad (\text{III.2})$$

with the boundary conditions

$$\begin{bmatrix} A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} C_{21} & C_{31} \\ C_{22} & C_{32} \\ C_{23} & C_{33} \end{bmatrix} = \begin{bmatrix} 0 & 0 \end{bmatrix} \quad (\text{III.2a})$$

Combining equations (III.1) and (III.1a)

$$\begin{bmatrix} (\alpha B_{11} - E_{22}) & \alpha B_{12} & \alpha B_{13} & -E_{23} & 0 & 0 \\ \alpha B_{21} & (\alpha B_{22} - E_{22}) & \alpha B_{23} & 0 & -E_{23} & 0 \\ A_{31} & A_{32} & (A_{33} + Bi) & 0 & 0 & 0 \\ -E_{32} & 0 & 0 & (\alpha B_{11} - E_{33}) & \alpha B_{12} & \alpha B_{13} \\ 0 & -E_{32} & 0 & \alpha B_{21} & (\alpha B_{22} - E_{33}) & \alpha B_{23} \\ 0 & 0 & 0 & A_{31} & A_{32} & (A_{33} + Bi) \end{bmatrix} \begin{bmatrix} T_{21} \\ T_{22} \\ T_{23} \\ T_{31} \\ T_{32} \\ T_{33} \end{bmatrix} = \begin{bmatrix} \beta g(T, C)_{21} + T_{11} E_{21} \\ \beta g(T, C)_{22} + T_{12} E_{21} \\ Bi T_C \\ \beta g(T, C)_{31} + T_{11} E_{31} \\ \beta g(T, C)_{32} + T_{12} E_{31} \\ Bi T_C \end{bmatrix} \quad (III.3)$$

Similarly for the mass balance equations

$$\begin{bmatrix} (\gamma B_{11} - E_{22}) & \gamma B_{12} & \gamma B_{13} & -E_{23} & 0 & 0 \\ \gamma B_{21} & (\gamma B_{22} - E_{22}) & \gamma B_{23} & 0 & -E_{23} & 0 \\ A_{31} & A_{32} & A_{33} & 0 & 0 & 0 \\ -E_{32} & 0 & 0 & (\gamma B_{11} - E_{33}) & \gamma B_{12} & \gamma B_{13} \\ 0 & -E_{32} & 0 & \gamma B_{21} & (\gamma B_{22} - E_{33}) & \gamma B_{23} \\ 0 & 0 & 0 & A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} C_{21} \\ C_{22} \\ C_{23} \\ C_{31} \\ C_{32} \\ C_{33} \end{bmatrix} = \begin{bmatrix} -g(T, C)_{21}/C_O + C_{11} E_{21} \\ -g(T, C)_{22}/C_O + C_{12} E_{21} \\ 0 \\ -g(T, C)_{31}/C_O + C_{11} E_{31} \\ -g(T, C)_{32}/C_O + C_{12} E_{31} \\ 0 \end{bmatrix} \quad (III.4)$$

The temperature and concentration at the start of each step are known so that the solution for the $(N+1) \times (M+1)$ unknown points of each step can be produced by iteratively solving the matrix equations (III.3) and (III.4) until the solution has converged. For the first step, the best initial estimate for the temperature and concentration is all $T=C=1$ i.e. the initial conditions of the dimensionless equations. After the first step, and for each successive step, the best estimate for the value of T and C at the new collocation points can be obtained by extrapolating the solution of the previous step using a modified form of equation (II.26)

$$T(z,r) = \sum_{i=1}^{M+2} d_i (1+z)^{i-1} \quad (\text{III.5})$$

If $M=1$ the solution for each step is a quadratic function of axial distance, with the overall solution consisting of interconnected quadratic arcs. Normally $N=2$ to 6 and $M=1$ or 2 so that excessive computer time is not used in evaluating the inverse of the left hand sides of equations (III.3) and (II.4), which are of rank $(M+1) \times (N+1)$ for the 1 phase model and twice this for the 2 phase model. These inverses, although slow to calculate using Gaussian elimination, or Crouts factorisation method, are only evaluated once and are then stored and re-used until the final solution to the complete reactor is obtained.

To solve the steady state heterogeneous model, equations (I.11) and (I.12) are treated similarly to the homogeneous model

$$St_{ht} \begin{bmatrix} (T_p - T_b)_{21} & (T_p - T_b)_{31} \\ (T_p - T_b)_{22} & (T_p - T_b)_{32} \\ (T_p - T_b)_{23} & (T_p - T_b)_{33} \end{bmatrix} = \beta \begin{bmatrix} g(T_p, C_p)_{21} & g(T_p, C_p)_{31} \\ g(T_p, C_p)_{22} & g(T_p, C_p)_{32} \\ g(T_p, C_p)_{23} & g(T_p, C_p)_{33} \end{bmatrix} \quad (III.5)$$

$$\begin{bmatrix} T_{b11} & T_{b21} & T_{b31} \\ T_{b12} & T_{b22} & T_{b32} \end{bmatrix} \begin{bmatrix} E_{21} & E_{31} \\ E_{22} & E_{32} \\ E_{23} & E_{33} \end{bmatrix} = St_{ht} \begin{bmatrix} (T_p - T_b)_{21} & (T_p - T_b)_{31} \\ (T_p - T_b)_{22} & (T_p - T_b)_{32} \end{bmatrix} + \alpha \begin{bmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \end{bmatrix} \begin{bmatrix} T_{b21} & T_{b31} \\ T_{b22} & T_{b32} \\ T_{b23} & T_{b33} \end{bmatrix} \quad (III.6)$$

with the boundary conditions

$$\begin{bmatrix} A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} T_{b21} & T_{b31} \\ T_{b22} & T_{b32} \\ T_{b23} & T_{b33} \end{bmatrix} = -Bi \begin{bmatrix} (T_{b23} - T_c) & (T_{b33} - T_c) \end{bmatrix} \quad (III.6a)$$

Similarly for the mass balance equations (I.13) and (I.14)

$$St_{mt} \begin{bmatrix} (C_p - C_b)_{21} & (C_p - C_b)_{31} \\ (C_p - C_b)_{22} & (C_p - C_b)_{32} \\ (C_p - C_b)_{23} & (C_p - C_b)_{33} \end{bmatrix} = -\frac{1}{C_o} \begin{bmatrix} g(T_p, C_p)_{21} & g(T_p, C_p)_{31} \\ g(T_p, C_p)_{22} & g(T_p, C_p)_{32} \\ g(T_p, C_p)_{23} & g(T_p, C_p)_{33} \end{bmatrix} \quad (III.7)$$

$$\begin{bmatrix} C_{b11} & C_{b21} & C_{b31} \\ C_{b12} & C_{b22} & C_{b32} \end{bmatrix} \begin{bmatrix} E_{21} & E_{31} \\ E_{22} & E_{32} \\ E_{23} & E_{33} \end{bmatrix} = St_{mt} \begin{bmatrix} (C_p - C_b)_{21} & (C_p - C_b)_{31} \\ (C_p - C_b)_{22} & (C_p - C_b)_{32} \end{bmatrix} + \gamma \begin{bmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \end{bmatrix} \begin{bmatrix} C_{b21} & C_{b31} \\ C_{b22} & C_{b32} \\ C_{b23} & C_{b33} \end{bmatrix} \quad (III.8)$$

with the boundary conditions

$$\begin{bmatrix} A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} C_{b21} & C_{b31} \\ C_{b22} & C_{b32} \\ C_{b23} & C_{b33} \end{bmatrix} = \begin{bmatrix} 0 & 0 \end{bmatrix} \quad (III.8a)$$

Combining equations (III.5), (III.6) and (III.6a)

$$\begin{bmatrix} (\alpha B_{11} - E_{11} - St_{ht}) & \alpha B_{12} & \alpha B_{13} & St_{ht} & 0 & 0 \\ \alpha B_{21} & (\alpha B_{22} - E_{22} - St_{ht}) & \alpha B_{23} & 0 & St_{ht} & 0 \\ A_{31} & A_{32} & (A_{33} + Bi) & 0 & 0 & 0 \\ -St_{ht} & 0 & 0 & St_{ht} & 0 & 0 \\ 0 & -St_{ht} & 0 & 0 & St_{ht} & 0 \\ 0 & 0 & -St_{ht} & 0 & 0 & St_{ht} \\ -E_{32} & 0 & 0 & 0 & 0 & 0 \\ 0 & -E_{32} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} T_{b21} & 0 & 0 & 0 & 0 & 0 \\ T_{b22} & 0 & 0 & 0 & 0 & 0 \\ T_{b23} & 0 & 0 & 0 & 0 & 0 \\ T_{p21} & 0 & 0 & 0 & 0 & 0 \\ T_{p22} & 0 & 0 & 0 & 0 & 0 \\ T_{p23} & 0 & 0 & 0 & 0 & 0 \\ T_{b31} & St_{ht} & 0 & 0 & 0 & 0 \\ T_{b32} & 0 & St_{ht} & 0 & 0 & 0 \\ T_{b33} & 0 & 0 & 0 & 0 & 0 \\ T_{p31} & St_{ht} & 0 & 0 & 0 & 0 \\ T_{p32} & 0 & St_{ht} & 0 & 0 & 0 \\ T_{p33} & 0 & 0 & St_{ht} & 0 & 0 \end{bmatrix} \begin{bmatrix} T_{b11} E_{21} \\ T_{b12} E_{21} \\ Bi T_C \\ \beta g(T_p, C)_{21} \\ \beta g(T_p, C)_{22} \\ \beta g(T_p, C)_{23} \\ T_{b11} E_{31} \\ T_{b12} E_{31} \\ Bi T_C \\ \beta g(T_p, C)_{31} \\ \beta g(T_p, C)_{32} \\ \beta g(T_p, C)_{33} \end{bmatrix}$$

(III.9)

Equations (III.7), (III.8) and (III.8a) for the heterogeneous mass balance equations are combined in an analogous manner to the energy balance equation (III.9).

To apply the orthogonal collocation method to the dynamic equations, where the concentration is assumed to be pseudo-steady state, the temperature partial derivative with respect to time, of equation (I.19), is replaced by a matrix equation derived in an analogous way to equation (II.32).

$$\frac{\partial T_p}{\partial t} = GT_p$$

Similarly to α and γ the dimensionless group ξ containing the heat capacity ratio must be modified by dividing by L , the number of axial collocation steps.

$$\xi = \frac{C_{p,p} \rho_p}{C_{p,g} \rho_g} \frac{Z}{t_r u L}$$

To allow variation of the time step a scaling factor T_s must be introduced into equation (I.19), modifying the dimensionless transformation to

$$\beta g(T_p, C_p) = St_{ht} (T_p - T_b) + \frac{\xi}{T_s} \frac{\partial T_p}{\partial t} \quad (III.10)$$

where $T_s = \frac{t}{t_r} \frac{1}{t_r}$

By increasing T_s the size of each collocation step in the time direction is increased.

Expressing the dynamic equation (III.10) in the collocation form similarly to the previous equations, with one internal collocation point in the time direction i.e. three

collocation points altogether, (identical to the axial collocation operation).

$$\beta \begin{bmatrix} g(T_p, C_p)_{2j1} & g(T_p, C_p)_{2j2} & g(T_p, C_p)_{2j3} \\ g(T_p, C_p)_{3j1} & g(T_p, C_p)_{3j2} & g(T_p, C_p)_{3j3} \end{bmatrix} = St_{ht} \begin{bmatrix} (T_p - T_b)_{2j1} & (T_p - T_b)_{2j2} & (T_p - T_b)_{2j3} \\ (T_p - T_b)_{3j1} & (T_p - T_b)_{3j2} & (T_p - T_b)_{3j3} \end{bmatrix} + \frac{\xi}{T_s} \begin{bmatrix} G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix} \begin{bmatrix} T_{b1j1} & T_{b1j2} & T_{b1j3} \\ T_{b2j1} & T_{b2j2} & T_{b2j3} \\ T_{b3j1} & T_{b3j2} & T_{b3j3} \end{bmatrix} \quad (III.11)$$

where $j=2,3$

Transforming equation (I.20)

$$\begin{bmatrix} T_{bi11} & T_{bi21} & T_{bi31} \\ T_{bi12} & T_{bi22} & T_{bi32} \end{bmatrix} \begin{bmatrix} E_{21} & E_{31} \\ E_{22} & E_{32} \\ E_{23} & E_{33} \end{bmatrix} = St_{ht} \begin{bmatrix} (T_p - T_b)_{i21} & (T_p - T_b)_{i31} \\ (T_p - T_b)_{i22} & (T_p - T_b)_{i32} \end{bmatrix} + \alpha \begin{bmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \end{bmatrix} \begin{bmatrix} T_{bi21} & T_{bi31} \\ T_{bi22} & T_{bi32} \\ T_{bi23} & T_{bi33} \end{bmatrix} \quad (III.12)$$

where $i=2,3$

with the reactor wall boundary conditions

$$\begin{bmatrix} A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} T_{bi21} & T_{bi31} \\ T_{bi22} & T_{bi32} \\ T_{bi23} & T_{bi33} \end{bmatrix} = -Bi \begin{bmatrix} (T_{bi23} - T_c) & (T_{bi33} - T_c) \end{bmatrix} \quad (III.12a)$$

where $i=2,3$

Combining the two matrix equations from each of equations (III.11) to (III.12a) results in the following set of 24 simultaneous equations.

To solve the matrix of equations for the transient case, the starting point is to solve the steady state equations for the heterogeneous model and store the temperature and concentration distributions. The variables to be changed are selected, the left hand side matrix of equation (III.9) is recalculated, unless only the inlet or bath temperatures are changed and inverted. The left hand side matrix of equation (III.13) is inverted, and the relevant boundary conditions imposed.

As the orthogonal collocation method in the axial direction consists of smoothly connected arcs, the overall function has a continuous first derivative. This means that the method does not lend itself easily to considering a discontinuity in the function as occurs over the space of one residence time interval immediately the inlet temperature or o-xylene concentration is stepwise changed. To overcome this, large time steps are used i.e. $T_s > 1$.

When the bath temperature or the gas flow rate is changed, the initial estimate of the temperature distribution along the length of the reactor for the first collocation step in the time direction is the same as the steady state temperature. The concentration however is pseudo-steady state so only the first axial collocation step in the time direction is estimated based on the original concentration distribution, unless the inlet concentration is changed, and then the concentration is extrapolated axially by equation (III.5) as for the steady state model. For the second and further time steps, the temper-

ature is best estimated by a modified form of equation (III.5) in which the extrapolation is of order N+1

$$T_p(t,z,r) = \sum_{i=1}^{M+2} d_i (1 + t)^{i-1} \quad (\text{III.14})$$

If the inlet temperature is changed, to estimate the temperature over the second time step near the inlet, equation (III.14) has to be reduced to the linear form due to the temperature discontinuity in the time direction.

Once the unknowns for each step have been estimated equation (III.13) and the heterogeneous steady state mass balance equation are iteratively solved until they converge. Note that the inverses of the left hand side matrices of these equations are constant for all time steps after the initial steady state.

Appendix IV

COLLOCATION MATRICES

Cylindrical Geometry

Collocation Points			Matrix A			Matrix B		
W = 1			W = 1-r ²			W = 1-r ²		
N=1	0.7071067812	0.5773502692	$\begin{bmatrix} -1.73205 & 1.73205 \\ -3 & 3 \end{bmatrix}$	$\begin{bmatrix} -6 & 6 \\ -6 & 6 \end{bmatrix}$	$\begin{bmatrix} -9.902381 & 12.299660 & -2.397279 \\ 9.033674 & -32.76486 & 23.730612 \\ 22.757482 & -65.424149 & 42.666667 \end{bmatrix}$	$\begin{bmatrix} -15.881426 & 19.636380 & -5.2811862 & 1.5262327 \\ 11.151861 & -34.497415 & 29.235709 & -5.8901550 \\ -3.5405872 & 34.512110 & -99.621159 & 68.649637 \\ -33.869987 & 136.24969 & -252.37970 & 150 \end{bmatrix}$		
N=2	0.4597008434	0.3937651911						
1	0.8880738340	0.8030871524						
N=3	0.3357106870	0.2976372952	$\begin{bmatrix} -2.539584 & 3.825616 & -1.286032 \\ -1.377677 & -1.245195 & 2.622872 \\ 1.715476 & -9.715476 & 8 \end{bmatrix}$	$\begin{bmatrix} -9.902381 & 12.299660 & -2.397279 \\ 9.033674 & -32.76486 & 23.730612 \\ 22.757482 & -65.424149 & 42.666667 \end{bmatrix}$	$\begin{bmatrix} -15.881426 & 19.636380 & -5.2811862 & 1.5262327 \\ 11.151861 & -34.497415 & 29.235709 & -5.8901550 \\ -3.5405872 & 34.512110 & -99.621159 & 68.649637 \\ -33.869987 & 136.24969 & -252.37970 & 150 \end{bmatrix}$			
1	0.7071067812	0.6398959794						
1	0.9419651451	0.8875018095						

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Planar Geometry

Collocation Points			Matrix A		Matrix B	
			$W = 1$		$W = 1$	
N=1	0		$\begin{bmatrix} -3 & 4 & -1 \\ -1 & 0 & 1 \\ 1 & -4 & 3 \end{bmatrix}$	$\begin{bmatrix} 4 & -8 & 4 \\ 4 & -8 & 4 \\ 4 & -8 & 4 \end{bmatrix}$		
N=2	0					
1	0.2113248654					
1	0.7886751346		$\begin{bmatrix} -7 & 8.196 & -2.196 & -1 \\ -2.732 & 1.732 & 1.732 & -0.7321 \\ 0.7321 & -1.732 & -1.732 & 2.732 \\ -1 & 2.196 & -8.196 & 7 \end{bmatrix}$	$\begin{bmatrix} 24 & -37.18 & 25.18 & -12 \\ 16.39 & -24 & 12 & -4.392 \\ -4.392 & 12 & -24 & 16.39 \\ -12 & 25.18 & -37.18 & 24 \end{bmatrix}$		

Cylindrical Geometry

Collocation Points

$W = 1$

$N = 4$	$N = 5$	$N = 6$
0.2634992300	0.2165873427	0.1837532119
0.5744645143	0.4803804169	0.4115766111
0.8185294874	0.7071067812	0.6170011402
0.9646596062	0.8770602346	0.7869622564
1	0.9762632447	0.9113751660
	1	0.9829724091
		1

$W = 1-r^2$

0.2389648430	0.1995240765	0.1712204053
0.5261587342	0.4449869862	0.3848098228
0.7639309081	0.6617966532	0.5805038245
0.9274913130	0.8339450062	0.7474433215
1	0.9494550617	0.8770597825
	1	0.9627801781
		1

Planar Geometry

Collocation Points

$W = 1$

$N = 1$	0.5	$N = 5$	0.0469100771
$N = 2$	0.2113248654		0.2307653450
	0.7886751346		0.5
$N = 3$	0.1127016654		0.7692346551
	0.5		0.9530899230
	0.8872983346	$N = 6$	0.0337652429
$N = 4$	0.0694318462		0.1693953068
	0.3300094783		0.3806904070
	0.6699905218		0.6193095931
	0.9305681558		0.8306046933
			0.9662347571

Note that the first collocation point $x_1=0$ and the last collocation point $x_{N+2}=1$.

Appendix V

LIST OF SYMBOLS

a	External surface area of pellet / empty tube volume	m^{-1}
Bi	Biot number ($h_w R/k_e$)	
C	Dimensionless o-xylene concentration	
C'	O-xylene concentration	$Kmole/m^3$
C _o	Inlet mole fraction o-xylene	
C' _o	Inlet o-xylene concentration	$Kmole/m^3$
C _{o₂}	Mole fraction oxygen	
C _{P_g}	Heat capacity of gas	$KJ/Kmole.^{\circ}C$
C _{P_p}	Heat capacity of catalyst pellet	$KJ/Kg.^{\circ}C$
C _r	Mole fraction aromatic reactant	
D	Diameter	m
D _e	Effective diffusivity	m^2/s
g(T,C)	Dimensionless rate of reaction	
G	Superficial Molar flux	$Kmole/m^2.s$
h	Heat transfer coefficient	$KJ/m^2.s.^{\circ}C$
ΔH _r	Heat of Reaction	$KJ/Kmole$
k _e	Effective radial conductivity	$KJ/m.s.^{\circ}C$
K _G	Pellet mass transfer coefficient	m/s
k _g	Conductivity of gas	$KJ/m.s.^{\circ}C$
k _r	Kinetic rate constant	$Kmole/m^3.s$
L	Number of axial collocation steps	
Nu	Nusselt number ($h_w D_p/k_g$)	
Pec	Peclet number ($D_p G/\epsilon \rho_g D_e$)	
Pr	Prandtl number ($C_p \mu/k_g$)	
r	Dimensionless radial distance	
r'	Radial distance	m
R	Radius of Reactor	m

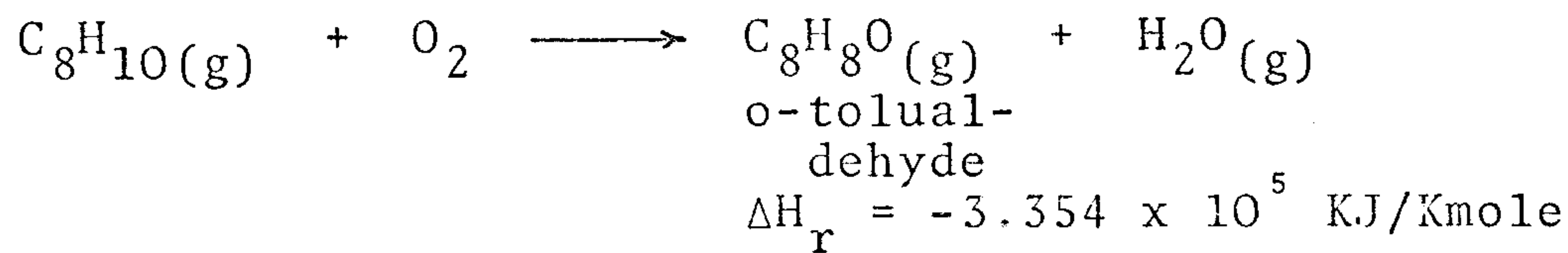
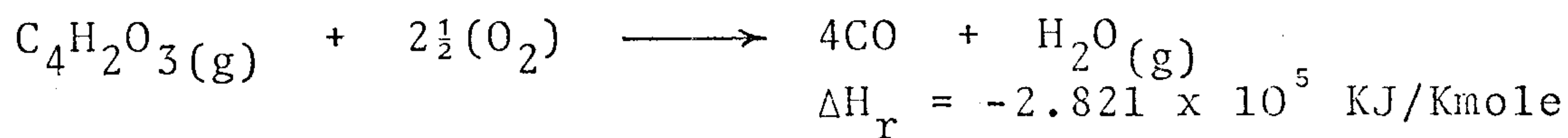
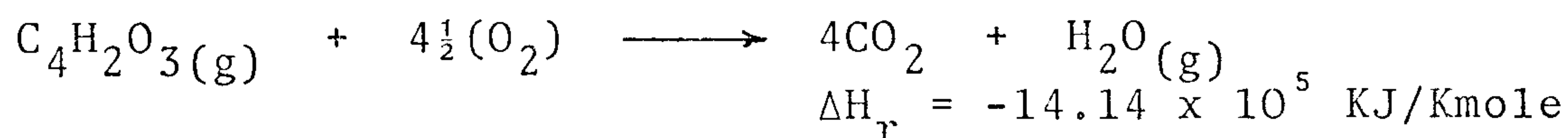
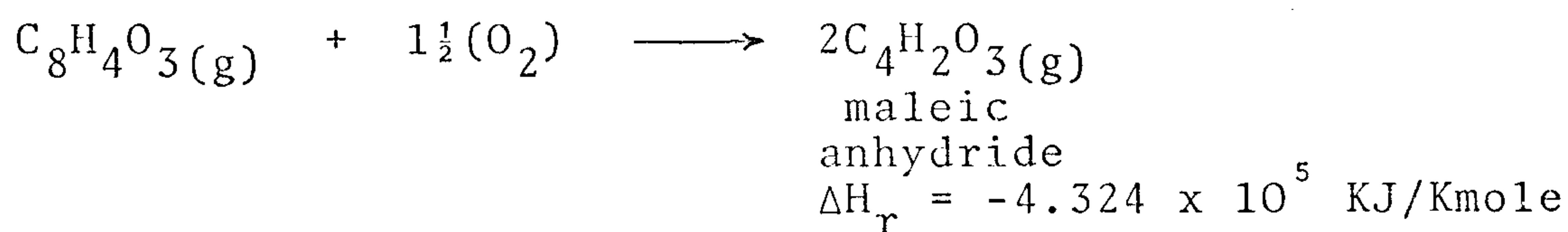
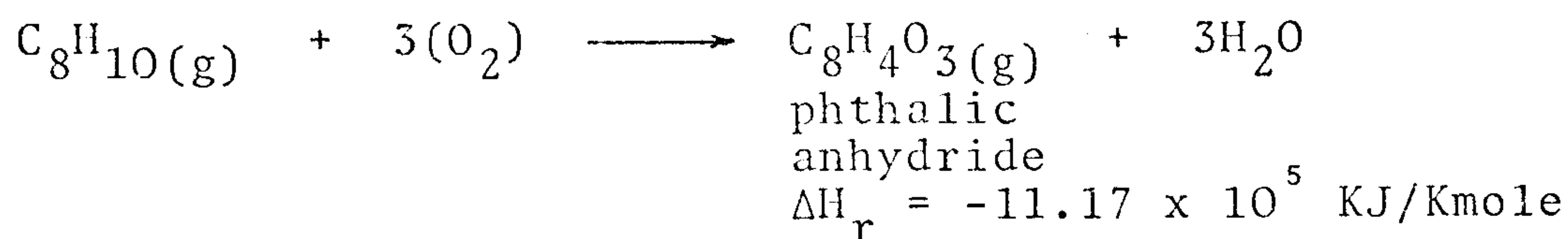
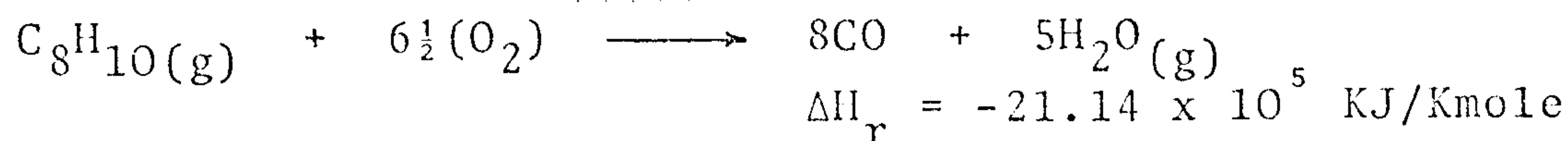
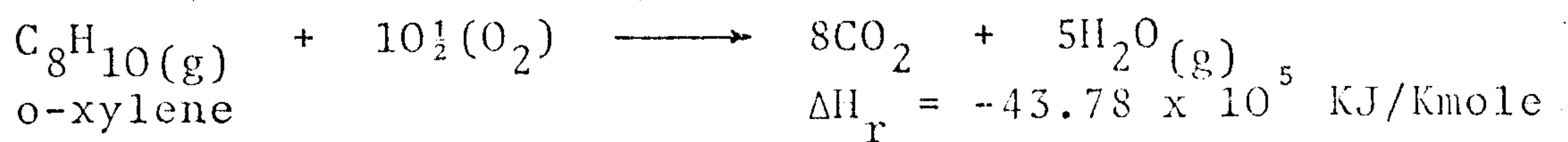
R_r	Rate of reaction	Kmole/m ³ .s
Re	Reynolds number ($D_p G/\mu$)	
Sc	Schmidt number ($\mu/\rho_f D_g$)	
St_{ht}	Modified Stanton number for heat transfer ($h_p aZ/C_{p_g} G$)	
St_{mt}	Modified Stanton number for mass transfer ($K_g aZ/u$)	
t	Dimensionless time	
t'	Time	s
T	Dimensionless temperature	
t_r	Gas residence time in reactor	s
u	Superficial gas velocity	m/s
U	Lumped heat transfer coefficient	KJ/m ² .s.°C
z	Dimensionless axial distance	
z'	Axial distance	m
Z	Reactor length	m
α	Dimensionless group ($k_e Z/C_{p_g} GR^2$)	
β	Dimensionless group ($-\Delta H_r/C_{p_g} \{\theta_o - \theta_{base}\}$)	
γ	Dimensionless group ($\epsilon D_e Z/R^2 u$)	
δ	Thickness of boundary layer on catalyst pellet	m
ϵ	Void fraction	
θ	Temperature	°C
ρ_g	Gas density	Kmole/m ³
ρ_p	Overall density of packed catalyst	Kg/m ³
μ	Viscosity	Kmole/m.s
ξ	Heat capacity ratio ($C_{p_p} \rho_p Z/C_{p_g} \rho_g t_r u$)	
T_s	Time scale factor	

Subscripts

b	Bulk gas
c	Coolant
o	Inlet
p	Pellet
t	Tube

Appendix VI

HEATS OF REACTION



Appendix VII

EXPERIMENTAL DATA

Run No.	Inlet Xylene Conc. (Mole%)	Gas Flow Rate (1/hr @ 25°C)	Inlet Temp. (°C)	P.A.	CO	CO ₂	Others	CO ₂ /CO Ratio	Unreacted Xylene	Overall ΔH_r (Kcal/gm mole xyl)
19A	0.313 0.394	480.4	346.8	80.4 80.0	5.00 4.93	13.2 13.4	1.4 1.6	2.67 2.84	<0.5 <0.5	-383.3 -384.7
19B	0.397 0.515	476.8	346.8	80.1 78.5	4.93 4.84	13.4 13.8	1.6 2.1	2.72 2.84	<0.5 0.80	-384.7 -388.7
21A	0.508 0.392	480.0	347.3	77.4 79.3	5.27 5.33	14.9 13.9	1.7 1.5	2.82 2.60	0.76 <0.5	-398.0 -389.1
21B	0.389 0.324	482.3	347.3	79.1 79.4	5.33 4.95	14.0 14.3	1.6 1.4	2.62 2.88	<0.5 <0.5	-390.0 -391.1
22A	0.452 0.335	398.6 478.0	348.25 348.0	78.4 79.4	5.36 5.19	14.9 14.0	1.4 1.4	2.78 2.70	<0.5 <0.5	-397.0 -389.8
22B	0.335 0.450	476.8 397.7	348.25 348.5	78.5 78.7	5.52 5.32	14.6 14.8	1.4 1.2	2.64 2.78	<0.5 <0.5	-395.0 -395.9
23A	0.507 0.444	370.4 403.9	346.8 346.6	77.3 77.4	5.56 5.80	15.2 14.8	1.5 1.6	2.74 2.55	0.38 0.44	-400.8 -398.1
23B	0.444 0.510	403.2 369.8	347.0 347.1	77.6 76.8	5.40 5.71	15.0 15.6	1.6 1.5	2.78 2.73	0.44 0.42	-398.8 -404.0
24B	0.619 0.465	402.7 482.8	340.6 340.6	46.8 53.5	2.74 3.42	9.68 10.8	6.8 6.6	3.53 3.15	34.0 25.7	-401.5 -399.5
24C	0.466 0.624	482.3 402.3	340.8 341.1	53.5 47.6	3.29 2.80	10.6 9.48	6.7 7.0	3.23 3.39	26.0 33.1	-398.5 -397.7

Run No.	Inlet Xylene Conc. (Mole%)	Gas Flow Rate (1/hr @ 25°C)	Inlet Temp. (°C)	P.A.	CO	CO ₂	Others	CO ₂ /CO Ratio	Unreacted Xylene	Overall ΔH_r (Kcal/gm mole xyl)
26A	0.640 0.545	436.7 483.5	349.7 349.7	76.4 76.6	5.79 5.87	15.3 14.7	1.9 1.9	2.65 2.51	0.64 0.98	-402.7 -398.8
27A	0.727 0.645	402.5 435.9	349.2 349.0	75.7 75.1	6.07 6.07	16.0 16.1	1.8 1.9	2.64 2.65	0.50 0.86	-408.3 -409.7
27B	0.635 0.529	436.6 483.5	349.7 349.4	75.6 76.4	6.07 5.78	16.1 15.0	1.7 1.9	2.65 2.60	0.60 0.89	-409.1 -400.8
28A	0.508 0.610	483.5 436.7	349.7 350.2	76.6 77.4	5.71 5.73	14.6 14.7	1.9 1.7	2.57 2.56	1.1 0.52	-397.9 -397.2
29A	0.459 0.362	483.3	346.3	62.7 75.6	4.56 4.86	12.9 14.1	5.6 3.0	2.84 2.91	14.2 2.5	-403.8 -394.9
29B	0.363 0.478	482.2	346.3	75.4 66.4	5.09 5.03	14.0 11.6	3.0 5.0	2.75 2.94	2.4 18.0	-394.2 -396.2
29C	0.464 0.568	482.0 435.3	346.3 346.6	67.6 63.2	4.40 3.88	13.4 12.7	4.6 5.5	3.05 3.27	9.9 14.8	-399.5 -400.0
29D	0.591 0.489	435.2 481.8	346.3 346.3	60.1 65.3	3.96 4.39	12.9 13.2	5.8 5.1	3.27 3.01	17.2 12.0	-407.1 -401.5
30A	0.524 0.477	476.8	351.7	76.9 78.1	5.49 5.01	14.9 14.3	2.0 2.0	2.71 2.85	0.75 0.64	-398.7 -392.9
30B	0.475 0.529	475.7	351.8	78.0 77.3	5.17 5.17	14.3 14.9	1.9 1.9	2.77 2.89	0.56 0.64	-393.4 -398.3
30C	0.531 0.647	475.7 429.6	352.1 352.3	77.3 77.2	5.39 5.49	14.6 15.0	2.0 1.9	2.71 2.74	0.66 0.40	-396.4 -399.3

Run No.	Inlet Xylene Conc. (Mole%)	Gas Flow Rate (1/hr @ 25°C)	Inlet Temp. (°C)	P.A.	CO	CO ₂	Others	CO ₂ /CO Ratio	Unreacted Xylene	Overall ΔH_r (Kcal/gm mole xyl)
32A	0.628	433.8	351.7	76.6	5.58	15.1	1.8	2.71	0.89	-401.0
	0.717	400.2	351.8	76.3	6.12	15.5	1.8	2.53	0.34	-404.3
32B	0.719	400.2	352.0	76.3	6.12	15.5	1.8	2.53	0.34	-404.3
	0.626	433.8	351.8	76.4	5.84	15.3	1.8	2.61	0.65	-402.3

[illegible]

TIME (min)	WATER	RAVING	TEMP	PELLET	2	3	4	5	6	7	8	9
0	349.09	349.02	346.82	343.47	371.37	381.82	375.41	363.28	357.08	353.74	350.64	348.25
1.00	349.09	350.16	346.82	349.47	371.13	381.82	375.41	363.28	357.32	353.50	350.40	348.01
2.00	349.25	350.16	346.82	349.47	371.13	381.82	375.41	363.28	357.32	353.74	350.40	348.01
3.00	349.01	349.02	346.82	349.47	371.13	381.82	375.41	363.28	357.32	353.74	350.64	348.01
4.00	349.09	350.40	346.82	349.47	371.13	381.82	375.41	363.28	357.32	353.50	350.40	348.01
5.00	349.25	350.40	346.82	349.47	371.13	381.82	375.41	363.28	357.32	353.50	350.40	348.01
6.00	349.09	349.92	346.82	349.47	370.18	389.89	385.86	369.51	362.09	357.08	352.55	349.97
7.00	349.25	349.92	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
8.00	349.09	350.64	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
9.00	349.25	349.92	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
10.00	349.09	349.92	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
11.00	349.25	349.92	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
12.00	349.09	350.64	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
13.00	349.25	350.64	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
14.00	349.09	349.92	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
15.00	349.25	350.64	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
16.00	349.09	349.92	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
17.00	349.25	349.92	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
18.00	349.09	350.64	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
19.00	349.25	350.64	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
20.00	349.09	350.64	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20
30.00	349.73	350.64	346.82	349.47	368.49	389.89	385.86	371.13	363.52	358.51	353.26	349.20

RUN 21A													
TIME (MIN)													
		RATH1	RATH2	INLET	PELLET	2	3	4	5	6	7	8	9
0		343.97	350.64	347.29	367.56	348.99	385.86	390.12	375.17	366.37	360.42	354.70	340.16
1.00		343.20	350.64	347.29	367.56	368.75	385.86	390.12	375.41	366.37	360.42	354.70	340.16
2.00		349.20	350.40	347.29	367.32	368.75	385.62	390.12	375.65	366.37	360.42	354.46	340.16
3.00		343.97	350.64	347.29	367.32	368.75	385.38	390.12	375.41	366.37	360.42	354.70	340.16
4.00		342.97	351.35	347.29	367.32	368.75	385.15	390.12	375.41	366.37	360.42	354.70	340.16
5.00		344.20	351.12	347.29	367.32	368.75	385.15	390.12	369.70	361.61	357.08	352.55	340.44
6.00		344.97	350.40	347.29	367.09	368.94	380.40	378.50	366.61	359.70	355.41	351.59	348.97
7.00		343.20	350.16	347.29	369.28	369.94	380.64	376.84	365.42	358.75	354.93	351.35	348.73
8.00		340.49	350.64	347.29	369.23	371.13	380.64	376.84	364.23	358.27	354.70	351.35	348.73
9.00		341.97	351.12	347.29	369.94	372.08	381.11	376.12	364.23	358.03	354.70	351.35	348.73
10.00		341.97	350.40	347.29	370.18	372.08	382.06	375.65	363.99	357.80	354.46	351.12	348.73
11.00		343.73	350.40	347.29	370.18	372.08	382.06	375.65	363.75	357.80	354.22	351.12	348.49
12.00		349.20	350.40	347.29	370.18	371.84	382.53	375.65	363.75	357.80	354.22	351.12	348.49
13.00		343.73	350.40	347.29	370.18	371.84	382.30	375.65	363.52	357.80	354.22	351.12	348.73
14.00		340.97	350.40	347.29	370.18	371.84	382.30	375.65	363.75	357.80	354.22	351.12	348.73
15.00		340.73	350.40	347.05	369.94	371.84	382.30	375.65	363.75	357.80	354.22	351.12	348.73
16.00		343.73	350.40	347.05	369.94	371.84	382.30	375.65	363.28	357.56	354.22	351.12	348.73
17.00		340.49	350.40	347.05	369.94	371.84	382.30	375.65	363.75	357.80	354.22	351.12	348.49
18.00		340.73	350.64	347.05	369.94	371.61	382.30	375.65	363.75	357.80	354.22	351.12	348.49
19.00		341.97	350.64	347.05	369.94	371.61	382.30	375.65	363.52	357.80	354.22	351.12	348.49
20.00		342.73	350.16	347.29	369.94	371.84	382.06	375.89	363.52	357.80	354.22	350.68	348.49
20.00		340.49	350.48	347.29	369.70	371.61	382.06	375.89	363.75	357.80	354.46	351.12	348.49

RUN 21B													
TIME (MIN)													
		RATH1	RATH2	INLET	PELLET	2	3	4	5	6	7	8	9
0		340.49	350.40	347.05	369.70	371.37	381.11	375.41	363.75	357.80	354.46	351.12	340.49
1.00		340.97	350.16	347.05	369.70	371.37	381.11	375.41	363.28	358.03	354.46	351.12	340.49
2.00		340.49	350.40	347.05	369.70	371.61	381.11	375.41	363.75	358.03	354.46	351.12	340.73
3.00		340.49	350.40	347.29	369.94	371.61	381.35	375.41	363.99	358.03	354.46	351.12	340.73
4.00		340.97	350.64	347.29	370.18	371.84	381.35	375.41	363.99	357.80	354.46	351.12	340.73
5.00		340.97	350.40	347.29	370.18	371.84	381.82	375.41	363.75	357.80	354.46	351.12	340.73
6.00		340.73	350.64	347.29	369.70	371.13	377.79	371.37	361.13	355.65	353.03	350.40	340.49
7.00		340.57	350.64	347.29	370.18	371.84	376.60	369.70	359.70	354.93	352.31	350.16	340.25
8.00		340.49	350.16	347.29	370.66	372.32	376.12	368.99	359.46	354.70	352.07	349.92	340.25
9.00		340.73	350.40	347.29	371.13	372.40	376.12	368.51	358.99	354.22	352.07	349.68	340.01
10.00		340.97	349.92	347.29	371.37	373.03	376.36	368.28	358.99	354.22	351.83	349.92	340.25
11.00		340.73	350.64	347.29	371.37	373.03	376.36	368.28	358.99	354.22	351.83	349.92	340.25
12.00		340.73	350.40	347.29	371.37	373.03	376.36	368.28	358.99	354.22	351.83	349.92	340.25
13.00		340.73	350.64	347.29	371.37	373.03	376.36	368.28	358.99	354.22	351.83	349.92	340.25
14.00		340.49	350.16	347.29	371.37	373.03	376.12	368.28	358.75	354.22	351.83	349.68	340.25
15.00		340.49	350.64	347.29	371.37	373.03	376.36	368.28	358.99	354.22	351.83	349.68	340.25
16.00		340.49	350.16	347.29	371.37	373.03	376.36	368.28	358.75	354.22	351.83	349.92	340.25
17.00		340.49	350.64	347.29	371.37	373.03	376.36	368.28	358.99	354.22	351.83	349.68	340.25
18.00		340.97	350.16	347.29	371.37	373.03	375.99	368.28	358.99	354.22	351.83	349.68	340.01
19.00		340.97	350.16	347.29	371.37	373.03	376.12	368.28	358.51	354.22	351.83	349.68	340.25
20.00		340.73	350.40	347.29	371.37	373.03	376.36	368.28	358.99	354.22	351.83	349.68	340.25
30.00		340.97	350.40	347.29	371.37	373.03	376.36	368.28	358.75	354.22	351.83	349.92	340.25

RUN 22A										
TIME (MIN)										
0	PATH1	PATH2	THLET	PELLET	2	3	4	5	6	7
1.00	349.44	351.12	348.25	376.36	378.97	387.99	374.93	361.13	355.65	352.79
2.00	349.44	350.88	348.25	376.36	378.97	387.99	374.70	361.13	355.65	352.79
3.00	349.49	350.64	348.25	376.36	378.74	387.75	374.93	360.89	355.65	352.79
4.00	349.44	351.59	348.25	376.36	378.97	388.23	375.17	361.37	355.89	352.79
5.00	349.20	350.88	348.25	376.36	378.97	387.99	374.93	361.13	355.65	352.79
5.08	349.44	351.12	348.25	376.36	378.97	388.23	374.93	361.61	355.89	352.79
5.17	349.64	350.88	348.01	375.89	377.79	387.28	375.17	361.85	355.89	353.03
5.25	349.64	350.64	348.01	375.89	377.79	387.28	374.70	361.61	355.89	353.03
5.33	349.64	351.12	348.01	375.89	377.31	386.57	374.46	361.37	355.65	352.79
5.42	349.22	350.88	348.01	374.70	376.84	386.09	374.22	361.37	355.65	352.79
5.50	349.42	350.88	348.01	374.70	376.36	385.86	374.22	361.37	355.65	352.79
5.58	349.64	350.64	348.01	374.46	376.12	385.38	373.98	361.37	355.65	352.79
5.67	349.64	351.12	348.01	373.75	375.65	384.67	373.75	361.13	355.65	352.79
5.75	349.64	350.88	348.01	373.51	375.65	384.20	373.51	360.89	355.41	352.79
5.83	349.64	350.64	348.01	373.51	375.17	383.48	373.27	360.66	355.41	352.79
5.92	349.42	350.88	348.01	373.51	375.17	383.25	373.03	360.89	355.41	352.55
6.00	349.92	350.88	348.01	373.03	374.93	383.01	372.80	360.89	355.41	352.55
6.08	349.42	350.88	348.01	373.03	374.70	382.77	372.80	360.89	355.41	352.55
6.17	349.44	350.88	348.01	372.80	374.46	382.30	372.56	360.89	355.17	352.55
6.25	349.64	350.88	348.01	372.56	374.22	381.59	372.32	360.42	355.17	352.55
6.33	349.44	350.64	348.01	372.56	374.22	381.35	372.08	360.18	355.17	352.55
6.42	349.44	350.64	348.01	372.32	374.22	380.97	371.84	360.18	355.17	352.55
6.50	349.42	350.64	348.01	372.32	373.98	380.47	371.84	360.18	355.17	352.55
6.58	349.64	350.64	348.01	372.08	373.75	380.16	371.84	360.18	355.17	352.55
6.67	349.44	350.64	348.01	372.08	373.75	379.92	371.61	360.18	355.17	352.55
6.75	349.44	350.88	348.01	372.08	373.75	379.92	371.61	360.42	354.93	352.55
6.83	349.64	350.88	348.01	372.08	373.75	379.92	371.37	360.18	355.17	352.55
6.92	349.44	350.64	348.01	371.84	373.51	379.45	371.37	360.18	354.93	352.55
7.00	349.44	350.64	348.01	371.84	373.51	379.21	371.37	360.18	354.93	352.55
7.08	349.64	351.12	348.01	371.84	373.51	379.21	371.37	360.18	354.93	352.55
7.17	349.64	351.12	348.01	371.84	373.51	379.21	371.13	360.18	354.93	352.55
7.25	349.64	350.64	348.01	371.84	373.51	378.97	371.13	360.42	354.93	352.55
7.33	349.44	351.12	348.01	371.84	373.51	378.97	371.13	360.42	354.93	352.55
7.42	349.44	351.12	348.01	371.84	373.51	378.97	371.13	360.42	355.17	352.55
7.50	349.44	351.12	348.01	371.84	373.51	378.97	371.13	360.42	355.17	352.55
7.58	349.20	350.64	348.01	371.84	373.51	378.97	371.13	360.18	355.17	352.55
7.67	349.44	351.12	348.01	371.84	373.51	378.97	371.13	360.18	355.17	352.55
7.75	349.20	351.12	348.01	371.84	373.51	378.97	371.13	360.18	355.17	352.55
7.83	349.64	350.88	347.77	371.61	373.27	378.26	370.89	360.42	355.17	352.55
7.92	349.44	351.12	347.77	371.61	373.27	378.26	370.89	360.42	355.17	352.55
8.00	349.44	351.12	347.77	371.61	373.27	378.26	370.89	360.42	355.17	352.55
8.08	349.44	351.12	348.01	371.84	373.27	378.26	370.89	360.18	355.17	352.55
8.17	349.20	351.12	347.77	371.61	373.27	377.79	370.66	360.18	355.17	352.55
8.25	349.20	351.12	347.77	371.61	373.27	378.02	370.66	360.18	355.17	352.55
8.33	349.20	351.12	348.01	371.61	373.27	378.02	370.66	360.42	355.17	352.55
8.42	349.20	350.64	347.77	371.61	373.27	377.79	370.66	360.18	355.17	352.55
9.00	349.64	350.64	347.77	371.37	373.03	377.31	370.42	360.18	355.17	352.79
10.00	349.97	351.12	347.77	371.37	373.03	377.31	370.42	360.18	355.17	352.79
11.00	349.97	350.64	347.77	371.37	373.03	376.84	370.18	360.18	355.17	352.79
12.00	349.20	351.35	347.77	371.61	373.27	376.60	369.94	360.42	355.41	352.79
13.00	349.20	351.12	347.77	371.61	373.27	376.84	369.94	360.42	355.41	352.79
14.00	349.20	351.12	347.77	371.61	373.03	376.84	369.94	360.18	355.41	352.79
15.00	349.44	351.12	347.77	371.61	373.03	376.84	369.94	360.18	355.41	352.79
16.00	349.97	350.88	347.77	371.61	373.03	376.84	369.94	360.18	355.41	352.79
17.00	349.20	350.88	347.77	371.61	373.27	377.07	369.94	360.18	355.41	352.79
18.00	348.97	350.88	347.77	371.61	373.27	376.84	369.94	360.42	355.41	352.79
19.00	348.97	350.64	347.77	371.61	373.27	376.60	369.94	360.18	355.41	352.79
20.00	349.20	350.88	347.77	371.61	373.27	376.84	369.94	360.42	355.41	352.79
20.00	349.73	351.12	347.77	371.61	373.27	376.84	369.94	360.18	355.41	352.79

RUN 22A									
TIME(MIN)									
0	FATH1	RATH2	INLET	PELLET	2	3	4	5	6
7	8	9	10	11	12	13	14	15	16
349.6A	350.40	34A.01	371.13	372.80	377.07	370.66	361.13	356.13	353.26
349.44	350.4A	34A.01	371.37	373.03	377.07	370.66	361.37	356.13	353.26
349.44	351.12	34A.25	371.37	373.03	377.07	370.66	361.13	356.13	353.26
349.44	351.35	34A.25	371.37	372.80	377.07	370.66	361.13	356.13	353.26
349.6A	350.48	34A.25	371.37	372.80	376.84	370.66	361.13	356.13	353.26
349.6A	351.12	34A.25	371.37	372.80	377.07	370.66	361.13	356.13	353.26
349.6A	351.12	34A.25	371.37	373.03	377.07	370.66	361.13	356.13	353.26
349.92	350.4A	34A.49	371.61	373.51	377.07	370.66	361.13	356.13	353.26
349.92	351.12	34A.49	371.84	373.9A	377.07	370.66	361.13	356.13	353.26
349.92	351.59	34A.49	372.08	374.22	378.26	371.13	361.13	356.13	353.26
349.92	350.4A	34A.49	372.56	374.70	378.74	371.61	361.37	356.13	353.26
349.6A	350.4A	34A.49	372.56	374.93	378.97	371.84	361.61	356.37	353.50
349.92	351.12	34A.49	373.03	375.17	379.45	372.08	361.61	356.37	353.50
349.92	351.12	34A.49	373.27	375.41	379.69	372.32	361.37	356.37	353.50
349.42	351.35	34A.49	373.27	375.65	380.16	372.56	361.85	356.60	353.50
349.6A	351.12	34A.25	373.51	375.65	380.16	372.80	361.61	356.60	353.50
349.44	351.12	34A.25	373.75	375.89	380.64	373.03	361.85	356.84	353.74
349.44	351.35	34A.25	373.75	376.12	381.11	373.03	362.32	356.84	353.74
349.44	351.35	34A.49	373.9A	376.12	381.35	373.51	362.56	356.84	353.74
349.44	350.64	34A.49	373.9A	376.36	381.59	373.51	362.32	357.08	353.74
349.6A	350.4A	34A.49	374.22	376.36	382.06	373.75	362.56	357.08	353.74
349.6A	350.4A	34A.49	374.22	376.60	381.82	373.75	362.56	357.08	353.74
349.44	351.35	34A.49	374.22	376.60	382.53	373.9A	362.56	357.08	353.74
349.6A	351.35	34A.49	374.46	376.84	382.53	374.22	362.80	357.32	353.74
349.6A	350.4A	34A.49	374.46	376.84	383.01	374.22	362.80	357.32	353.74
349.16	350.4A	34A.49	374.46	376.84	382.77	374.46	362.80	357.32	353.74
349.92	351.12	34A.49	374.70	376.84	383.25	374.46	362.80	357.32	353.74
349.92	350.4A	34A.25	374.70	377.07	383.25	374.46	363.04	357.32	353.74
349.6A	350.4A	34A.25	374.70	377.07	383.48	374.46	363.04	357.32	353.74
349.92	350.4A	34A.25	374.70	377.07	383.48	374.70	363.04	357.32	353.74
349.92	351.12	34A.25	374.70	377.07	384.43	374.93	363.04	357.32	353.74
349.6A	351.12	34A.49	374.70	377.07	384.43	374.93	363.04	357.32	353.74
349.44	351.12	34A.49	374.70	377.07	384.67	374.93	362.80	357.32	353.74
349.6A	351.12	34A.49	374.93	374.93	384.67	374.93	363.04	357.32	353.74
349.6A	350.4A	34A.49	374.93	374.93	384.67	375.17	363.04	357.32	353.74
349.44	350.4A	34A.49	374.93	374.93	384.91	375.17	363.04	357.32	353.74
349.6A	350.4A	34A.49	374.93	374.93	385.15	375.17	363.04	357.32	353.74
349.6A	351.12	34A.49	374.93	374.93	385.15	375.17	363.04	357.32	353.74
349.44	351.59	34A.49	374.93	374.93	385.38	375.17	363.04	357.32	353.74
349.44	351.35	34A.49	374.93	374.93	385.38	375.41	362.80	357.32	353.74
349.6A	351.12	34A.49	374.93	374.93	385.38	375.41	362.80	357.32	353.74
349.6A	351.12	34A.25	374.93	374.93	385.38	375.41	362.80	357.32	353.74
349.6A	351.35	34A.49	374.93	374.93	385.62	375.41	362.56	357.08	353.50
349.92	350.64	34A.49	374.93	374.93	385.86	375.41	362.56	357.08	353.50
349.92	351.35	34A.49	374.93	374.93	386.33	375.41	362.32	356.84	353.74
349.6A	351.35	34A.49	374.93	374.93	387.04	375.65	362.32	356.60	353.50
349.6A	350.4A	34A.49	374.93	374.93	387.04	375.89	361.85	356.60	353.26
349.92	351.59	34A.25	374.93	374.93	387.52	375.89	362.09	356.60	353.50
349.92	351.35	34A.25	374.93	374.93	387.52	375.89	362.56	356.37	353.26
349.44	351.35	34A.25	374.93	374.93	387.75	376.12	362.56	356.60	353.26
349.6A	351.35	34A.25	374.93	374.93	387.75	376.12	362.56	356.60	353.26
349.20	351.59	34A.25	374.93	374.93	387.99	375.89	362.32	356.13	353.26
349.6A	351.12	34A.49	374.93	374.93	387.99	375.89	361.85	356.13	353.26
349.6A	350.64	34A.49	375.17	375.17	387.52	375.89	362.09	356.37	353.26
349.92	351.12	34A.49	375.17	375.17	387.52	375.89	362.32	356.37	353.26
349.6A	350.4A	34A.49	375.17	375.17	387.75	375.89	362.56	356.37	353.26
349.6A	351.12	34A.49	375.17	375.17	387.75	375.89	362.56	356.37	353.26
30.00	349.44	351.12	375.17	375.17	387.75	375.89	362.09	356.37	353.26

TIME (MIN)	PATH1	RATH2	THLET	PELLET	2	3	4	5	6	7	8	9
0												
1.00	348.44	349.44	346.82	371.84	374.46	391.31	379.45	362.80	355.89	352.07	349.20	347.20
2.00	347.29	349.20	346.82	372.32	374.70	391.55	378.97	362.32	355.89	352.07	349.44	347.20
3.00	347.77	349.92	347.05	372.32	374.93	391.55	378.97	362.80	355.89	352.07	349.68	347.53
4.00	348.25	349.20	346.82	372.08	374.46	391.55	378.97	362.32	355.89	352.31	349.44	347.53
5.00	348.25	349.92	346.82	371.61	374.22	391.78	378.97	362.80	355.89	352.31	349.44	347.53
5.08	348.25	350.16	346.82	371.61	373.98	391.78	378.97	362.56	356.13	352.31	349.44	347.53
5.17	348.25	350.16	346.82	371.61	373.98	392.02	378.97	362.56	356.13	352.31	349.44	347.53
5.25	348.25	349.92	346.82	371.61	373.98	391.78	378.97	362.56	356.13	352.31	349.44	347.53
5.33	348.25	349.44	346.82	371.37	373.75	391.55	378.97	362.56	356.13	352.31	349.44	347.53
5.42	348.25	349.92	346.82	371.13	373.51	391.55	378.97	362.80	356.13	352.31	349.44	347.53
5.50	348.25	349.44	346.82	370.89	373.27	391.07	378.97	362.80	356.13	352.31	349.44	347.53
5.58	348.25	349.44	346.82	370.89	373.03	390.60	378.97	362.56	356.13	352.31	349.44	347.53
5.67	348.25	349.44	346.82	370.66	372.80	390.60	378.97	362.56	356.13	352.31	349.44	347.53
5.75	348.25	349.20	346.82	370.42	372.80	389.89	378.97	362.32	356.13	352.31	349.44	347.53
5.83	348.01	349.44	346.82	370.42	372.56	389.41	378.97	362.56	355.89	352.31	349.44	347.53
5.92	348.01	349.20	346.82	370.18	372.32	389.41	378.97	362.56	355.89	352.31	349.44	347.53
6.00	348.01	349.44	346.82	370.18	372.32	389.41	378.97	362.32	355.89	352.31	349.44	347.53
6.08	348.01	349.20	346.82	369.94	372.32	388.23	377.79	362.32	355.89	352.31	349.44	347.53
6.17	348.25	349.20	346.82	369.94	372.32	388.23	377.79	362.56	355.89	352.31	349.44	347.53
6.25	348.25	349.44	346.82	369.94	372.08	387.52	377.55	362.09	355.89	352.31	349.44	347.53
6.33	348.25	349.44	346.82	369.94	372.08	387.52	377.55	362.32	355.89	352.31	349.44	347.53
6.42	348.25	349.44	346.82	369.70	372.08	387.52	377.55	362.09	355.89	352.31	349.44	347.53
6.50	348.25	349.44	346.82	369.70	372.08	387.52	377.55	362.56	355.89	352.31	349.44	347.53
6.58	348.25	349.92	346.82	369.70	371.84	387.04	377.55	362.56	355.89	352.31	349.44	347.53
6.67	348.25	349.20	346.82	369.70	371.84	386.81	377.55	362.32	355.89	352.31	349.44	347.53
6.75	348.01	349.92	346.82	369.70	371.84	386.81	377.55	362.56	355.89	352.31	349.44	347.53
6.83	348.25	349.20	346.82	369.70	371.84	386.81	377.55	362.09	355.89	352.31	349.44	347.53
6.92	348.25	349.20	346.82	369.70	371.84	386.33	377.31	362.09	355.89	352.31	349.44	347.53
7.00	348.25	348.73	346.82	369.70	371.84	386.33	377.31	362.56	355.89	352.31	349.44	347.53
7.08	348.25	348.73	346.82	369.70	371.84	386.09	377.31	362.56	355.89	352.31	349.44	347.53
7.17	348.25	348.97	346.82	369.70	371.84	385.86	377.31	362.56	355.89	352.31	349.44	347.53
7.25	348.25	348.97	346.82	369.70	371.84	385.62	377.31	362.32	355.89	352.07	349.44	347.53
7.33	348.01	348.97	346.82	369.47	371.84	385.62	377.31	362.56	355.89	352.07	349.44	347.53
7.42	348.01	348.97	346.82	369.47	371.84	385.62	377.31	362.56	355.89	352.07	349.44	347.53
7.50	347.77	348.97	346.82	369.47	371.61	385.38	377.31	362.56	355.89	352.07	349.44	347.53
7.58	347.77	349.20	346.82	369.70	371.84	385.38	377.31	362.56	355.89	352.07	349.44	347.53
7.67	348.01	348.97	346.82	369.70	371.61	385.15	377.31	362.56	355.89	352.07	349.44	347.53
7.75	348.01	349.20	346.82	369.70	371.84	384.91	377.07	362.56	355.89	352.07	349.44	347.53
7.83	348.25	348.97	346.82	369.47	371.61	384.91	377.07	362.56	355.89	352.07	349.44	347.53
7.92	348.01	349.20	346.82	369.70	371.61	384.91	377.07	362.56	355.89	352.07	349.44	347.53
8.00	349.01	349.20	346.82	369.70	371.61	384.67	377.07	362.56	355.89	352.31	349.44	347.53
8.08	348.01	349.20	346.82	369.70	371.61	384.43	377.07	362.32	355.89	352.07	349.44	347.53
8.17	348.25	349.20	346.82	369.70	371.61	384.43	377.07	362.56	355.89	352.31	349.44	347.53
8.25	348.25	348.97	346.82	369.47	371.61	384.43	376.84	362.80	355.89	352.31	349.44	347.53
8.33	348.25	349.20	346.82	369.47	371.61	384.20	376.84	362.80	355.89	352.31	349.44	347.53
8.42	348.25	349.44	346.82	369.47	371.84	384.20	376.84	362.80	355.89	352.31	349.44	347.53
9.00	348.25	349.20	346.82	369.70	371.84	383.48	376.84	363.04	356.13	352.31	349.44	347.53
10.00	348.25	348.73	346.82	369.70	371.84	383.01	376.60	362.80	356.37	352.55	349.44	347.53
11.00	347.77	349.44	346.82	369.94	372.08	383.01	376.36	362.80	356.37	352.55	349.44	347.53
12.00	348.25	349.20	346.82	369.94	372.08	382.77	376.36	363.28	356.60	352.55	349.44	347.53
13.00	348.25	349.20	346.82	370.18	372.32	382.53	376.12	363.04	356.84	352.55	349.44	347.29
14.00	348.25	349.68	346.82	370.18	372.32	383.01	376.12	363.04	356.84	352.55	349.44	347.53
15.00	348.25	350.40	346.82	370.18	372.32	383.01	376.12	363.28	356.84	352.79	349.44	347.29
16.00	348.01	349.92	346.82	370.18	372.32	382.77	375.89	362.80	356.60	352.79	349.44	347.29
17.00	348.01	349.20	346.82	370.18	372.32	382.77	375.89	363.04	356.60	352.79	349.44	347.29
18.00	348.01	349.92	346.82	370.18	372.32	382.77	375.89	363.04	356.60	352.55	349.44	347.29
19.00	348.25	349.92	346.82	370.18	372.32	383.01	375.89	363.04	356.60	352.55	349.44	347.29
20.00	348.01	350.16	346.82	369.94	372.32	383.25	375.89	363.28	356.60	352.55	349.44	347.29
30.00	348.01	348.73	346.82	369.47	371.61	382.30	376.12	363.04	356.84	352.55	349.20	347.29

TIME (MIN)	RATH1	RATH2	INLET	PELLET	2	3	4	5	6	7	8	9
0	348.25	350.16	346.82	370.42	372.56	383.48	375.89	362.80	356.60	353.03	349.92	348.01
1.00	346.25	350.16	346.82	370.18	372.32	383.25	376.12	362.80	356.60	353.03	350.16	347.77
2.00	348.49	350.16	347.05	370.18	372.32	383.25	376.12	363.04	356.84	353.03	349.92	347.77
3.00	348.49	349.92	346.82	370.18	372.32	383.01	376.36	363.04	356.84	353.03	349.68	347.53
4.00	348.25	350.16	347.05	370.42	372.56	383.01	376.36	363.28	356.84	353.03	349.92	347.77
5.00	346.25	349.44	347.05	370.66	372.56	383.25	376.12	363.52	356.84	353.03	349.92	347.77
5.08	348.49	349.68	346.82	370.66	372.80	383.72	376.12	363.04	356.84	353.03	349.92	347.77
5.17	348.49	349.68	347.05	370.89	373.27	383.48	376.36	363.28	356.84	353.03	349.92	347.77
5.25	348.49	349.68	347.05	371.13	373.51	383.96	376.60	363.04	356.84	353.03	349.92	347.77
5.42	348.44	349.68	347.05	371.13	373.51	384.20	376.60	363.28	356.84	353.03	349.92	347.77
5.50	348.73	349.68	347.05	371.37	373.75	384.67	376.84	363.28	356.84	353.03	349.92	347.77
5.58	348.73	349.44	347.05	371.37	373.75	384.67	376.84	363.52	356.84	353.03	349.92	347.77
5.67	348.73	349.20	347.05	371.61	373.98	385.15	377.31	363.75	356.84	353.03	350.16	347.77
5.75	348.49	349.20	347.05	371.61	373.98	385.38	377.31	363.52	357.08	353.03	350.16	347.77
5.83	348.73	349.44	347.05	371.61	374.22	385.38	377.55	363.75	357.08	353.03	349.92	347.77
5.92	348.73	349.20	347.05	371.84	374.22	385.62	377.55	363.75	357.08	353.03	349.92	347.77
6.00	348.73	349.20	347.05	371.84	374.22	385.86	377.79	363.52	357.08	353.03	350.16	347.77
6.08	348.73	349.44	347.05	371.84	374.22	386.09	377.79	363.99	357.08	353.03	349.92	347.77
6.17	348.73	349.44	347.05	371.84	374.46	386.09	378.02	363.75	357.08	353.03	349.92	347.77
6.25	348.49	349.92	347.05	371.84	374.46	386.81	378.02	363.99	357.32	353.03	350.16	347.77
6.33	348.49	349.68	347.05	372.08	374.46	386.81	378.02	364.23	357.32	353.03	350.16	347.77
6.42	348.49	349.44	347.05	372.08	374.46	387.04	378.02	363.99	357.32	353.03	349.92	347.77
6.50	348.49	349.44	347.05	372.08	374.70	387.28	378.26	363.99	357.32	353.03	349.92	347.77
6.58	348.49	349.20	347.05	372.08	374.70	387.52	378.50	363.99	357.32	353.03	350.16	347.77
6.67	348.49	349.44	347.05	372.08	374.70	387.52	378.50	363.99	357.32	353.03	349.92	347.77
6.75	348.49	349.20	347.05	372.08	374.70	387.75	378.50	363.99	357.32	353.03	350.16	347.77
6.83	348.49	349.20	347.05	372.08	374.70	387.99	378.50	363.99	357.32	353.03	349.92	347.77
6.92	348.73	349.20	347.05	372.08	374.70	387.99	378.50	363.99	357.32	353.03	350.16	347.77
7.00	348.49	349.44	347.05	372.32	374.70	387.99	378.50	363.99	357.32	353.03	350.16	347.77
7.08	348.73	349.44	347.05	372.32	374.70	388.47	378.50	364.23	357.08	353.03	350.16	347.77
7.17	348.73	349.44	347.05	372.32	374.70	388.47	378.74	364.23	357.08	353.03	350.16	347.77
7.25	348.49	349.20	347.05	372.32	374.93	388.47	378.74	364.23	357.08	353.03	350.16	347.77
7.33	348.73	349.20	347.05	372.32	374.93	388.70	378.97	363.99	357.08	353.03	349.92	347.77
7.42	348.49	349.44	347.05	372.32	374.93	388.47	378.74	363.52	356.84	352.79	349.92	347.77
7.50	348.73	349.44	347.05	372.32	374.93	389.18	378.74	364.23	356.84	352.79	350.16	348.01
7.58	348.73	349.20	347.05	372.32	374.93	389.18	378.97	364.23	356.84	352.79	349.92	347.77
7.67	348.73	349.20	347.05	372.32	374.93	389.18	378.97	363.99	356.84	352.79	349.92	347.77
7.75	348.73	349.20	347.05	372.32	374.93	389.41	378.97	363.99	356.84	352.79	349.92	347.77
7.83	348.73	349.44	347.05	372.32	374.93	389.41	378.97	363.52	356.84	352.79	349.92	347.77
7.92	348.73	349.44	347.05	372.32	374.93	389.65	378.97	363.75	356.60	352.79	349.92	347.77
8.00	348.73	349.68	347.05	372.32	374.93	389.49	378.97	363.75	356.60	352.55	349.92	347.77
8.08	348.73	349.68	347.05	372.32	374.93	389.89	378.97	363.99	356.60	352.55	349.92	347.77
8.17	348.49	349.68	347.05	372.56	374.93	389.89	378.97	364.23	356.60	352.55	349.92	347.77
8.25	348.49	349.44	347.05	372.56	375.17	390.12	378.97	363.99	356.60	352.55	349.92	347.77
8.33	348.73	349.68	347.05	372.56	375.17	390.12	378.97	363.52	356.60	352.55	349.68	347.53
8.42	348.49	349.44	347.05	372.56	375.17	390.36	378.97	363.75	356.60	352.55	349.68	347.53
9.00	348.49	349.44	347.05	372.56	375.17	390.44	379.21	363.28	356.60	352.55	349.44	347.53
10.00	348.49	349.68	347.05	372.56	375.17	391.78	379.21	363.28	356.37	352.31	349.44	347.53
11.00	348.49	349.68	347.05	372.56	375.41	392.26	379.21	363.28	356.37	352.31	349.68	347.53
12.00	348.49	349.92	347.05	372.56	375.17	392.73	379.21	362.80	356.13	352.31	349.44	347.53
13.00	348.49	349.68	347.05	372.56	375.17	392.73	379.21	363.04	356.13	352.31	349.44	347.77
14.00	348.73	349.44	347.05	372.56	375.17	392.97	379.45	362.80	356.13	352.07	349.44	347.77
15.00	348.73	349.44	347.05	372.56	375.17	392.97	379.45	362.80	355.89	352.07	349.68	347.77
16.00	348.49	349.44	347.05	372.56	375.17	393.21	379.45	362.56	356.13	352.07	349.44	347.53
17.00	348.49	350.16	347.29	372.56	375.41	393.21	379.45	363.04	356.13	352.31	349.44	347.53
18.00	348.49	350.40	347.29	372.80	375.41	393.21	379.45	362.56	356.13	352.55	349.20	347.53
19.00	348.49	349.44	347.29	372.80	375.41	392.97	379.45	362.80	356.13	352.31	349.44	347.53
20.00	348.97	349.44	347.29	372.80	375.41	393.21	379.45	362.80	355.89	352.07	349.44	347.77
30.00	348.73	349.44	347.05	373.03	375.89	393.44	379.21	361.85	355.17	351.83	349.44	347.53

TIME (MIN)	BATH1	BATH2	INLET	PELLET	2	3	4	5	6	7	8	9
0	342.27	343.95	340.84	350.88	351.59	352.79	353.50	353.50	355.41	358.27	356.37	350.40
1.00	342.03	344.43	340.84	350.88	351.59	353.03	353.26	353.50	355.41	358.27	356.60	350.64
2.00	342.51	343.95	340.60	350.88	351.59	353.03	353.26	353.50	355.65	358.51	356.84	350.64
3.00	342.51	343.95	340.60	350.88	351.59	353.03	353.26	353.50	355.65	358.27	356.60	350.64
4.00	342.03	343.95	340.60	350.88	351.59	353.26	353.26	353.50	355.65	358.27	356.60	350.40
5.00	342.27	344.66	340.84	350.88	351.59	353.03	353.50	353.74	355.65	358.27	356.60	350.64
5.08	342.27	344.66	340.84	350.88	351.59	353.03	353.50	353.98	355.65	358.51	356.84	350.64
5.17	342.51	344.66	341.08	351.12	352.07	353.50	353.74	353.98	355.89	358.75	356.84	350.64
5.25	342.27	344.43	341.08	351.12	352.07	353.50	353.98	353.98	356.13	358.99	357.08	350.64
5.33	342.27	344.43	341.08	351.12	352.07	353.50	353.98	353.98	356.13	358.99	357.32	350.64
5.42	342.51	344.43	341.08	351.35	352.31	353.26	353.98	353.98	356.37	359.23	357.56	350.88
5.50	342.51	344.43	341.08	351.35	352.07	353.26	353.98	353.74	356.60	359.46	357.56	350.88
5.58	342.51	344.43	341.08	351.35	352.31	353.50	353.98	353.98	356.60	359.46	357.80	350.88
5.67	342.51	343.95	341.08	351.35	352.31	353.50	353.98	353.74	356.60	359.46	357.80	350.88
5.75	342.27	343.47	341.08	351.35	352.31	353.50	353.98	353.74	356.60	359.46	357.80	350.88
5.83	342.51	343.71	341.08	351.35	352.31	353.50	353.98	353.74	356.60	359.70	357.80	351.12
5.92	342.51	343.71	341.08	351.35	352.31	353.50	353.98	353.74	356.60	359.70	358.03	351.12
6.00	342.51	343.95	341.08	351.35	352.31	353.50	353.98	353.74	356.60	359.70	357.80	351.35
6.08	342.51	344.43	341.08	351.35	352.31	353.50	353.98	354.46	356.60	359.70	358.03	351.35
6.17	342.51	344.19	341.08	351.59	352.31	353.50	353.98	353.98	356.60	359.70	358.03	351.59
6.25	342.51	344.43	341.08	351.35	352.31	353.74	353.98	353.98	356.60	359.70	358.03	351.59
6.33	342.51	344.66	341.08	351.35	352.31	353.50	353.98	353.98	356.60	359.70	358.03	351.59
6.42	342.51	343.71	341.08	351.35	352.31	353.50	353.98	353.98	356.60	359.70	358.03	351.59
6.50	342.51	343.71	341.08	351.59	352.31	353.50	353.74	353.98	356.37	359.70	358.03	351.59
6.58	342.51	343.71	341.08	351.35	352.31	353.74	353.98	354.22	356.60	359.70	358.03	351.59
6.67	342.75	343.95	341.08	351.35	352.31	353.26	353.74	353.74	356.37	359.70	358.03	351.59
6.75	342.27	344.19	341.08	351.35	352.31	353.26	353.74	353.74	356.37	359.70	358.03	351.59
6.83	342.27	343.71	341.08	351.35	352.31	353.26	353.74	353.98	356.37	359.70	358.03	351.59
6.92	342.27	343.95	341.08	351.35	352.31	353.26	353.74	353.98	356.37	359.46	357.80	351.59
7.00	342.27	344.19	341.08	351.35	352.07	353.26	353.74	353.74	356.37	359.46	357.80	351.83
7.08	342.27	343.71	341.08	351.35	352.31	353.50	353.74	353.74	356.37	359.46	358.03	351.83
7.17	342.27	343.95	341.08	351.35	352.07	353.50	353.74	353.74	356.13	359.46	358.03	351.59
7.25	342.27	343.95	341.08	351.35	352.07	353.26	353.74	353.74	356.13	359.46	357.80	351.83
7.33	342.27	344.19	341.08	351.35	352.07	353.26	353.74	353.74	356.13	359.46	357.80	351.83
7.42	342.27	344.43	341.08	351.35	352.07	353.03	353.50	353.26	356.13	359.23	357.80	351.59
7.50	342.27	344.19	341.08	351.35	352.31	353.26	353.74	353.74	356.13	359.23	357.80	351.83
7.58	342.27	344.19	341.08	351.35	352.07	353.26	353.50	353.50	356.13	359.23	357.80	351.83
7.67	342.27	344.19	341.08	351.35	352.07	353.26	353.50	353.50	356.13	359.23	357.80	351.83
7.75	342.03	344.19	341.08	351.35	352.07	353.26	353.50	353.74	355.89	359.23	357.80	351.83
7.83	342.27	344.43	341.08	351.35	352.07	353.03	353.50	353.50	355.89	359.23	357.56	351.83
7.92	342.03	344.43	341.08	351.35	352.07	353.03	353.50	353.26	355.89	359.99	357.56	351.59
8.00	342.27	344.19	341.08	351.35	352.07	352.79	353.50	353.03	355.89	359.99	357.56	351.59
8.08	342.27	344.43	341.08	351.35	352.07	353.03	353.74	353.74	355.89	359.99	357.56	351.83
8.16	342.27	344.66	341.08	351.35	352.07	353.03	353.26	353.26	355.65	359.75	357.32	351.59
9.00	342.51	344.19	341.08	351.12	352.07	353.03	353.26	353.26	355.65	359.51	357.08	351.59
10.00	342.51	344.19	341.08	351.12	352.07	353.03	353.26	353.26	355.65	359.51	356.84	351.59
11.00	342.51	343.95	341.08	351.12	352.07	353.03	353.26	353.26	355.41	359.51	356.84	351.59
12.00	342.51	343.71	341.08	351.12	352.07	352.79	353.26	353.26	355.17	359.27	356.84	351.35
13.00	342.27	343.95	341.08	351.35	352.07	352.79	353.26	353.03	355.17	359.27	356.84	351.35
14.00	342.51	344.43	341.08	351.35	352.07	352.79	353.26	353.03	355.17	359.27	356.84	351.35
15.00	342.51	344.66	341.32	351.12	352.07	353.03	353.26	353.26	355.41	359.51	356.60	351.12
16.00	342.75	344.43	341.32	351.35	352.07	353.26	353.26	353.50	355.65	359.51	356.60	351.12
17.00	342.51	343.95	341.08	351.35	352.31	353.03	353.26	353.26	355.41	359.51	356.84	351.12
18.00	342.51	344.43	341.08	351.35	352.31	353.03	353.26	353.50	355.41	359.51	357.08	351.35
19.00	342.27	344.43	341.32	351.35	352.07	353.03	353.26	353.26	355.41	359.51	356.84	351.35
20.00	342.51	343.71	341.08	351.35	352.31	353.03	353.26	353.26	355.41	359.51	356.84	351.35
30.00	342.51	344.66	341.08	351.35	352.31	353.03	353.26	353.26	355.41	359.75	356.84	351.35

RUN 26A TIME (MIN)	DATA1	RATIO2	TULFT	PELLET	2	3	4	5	6	7	8	9
0	351.35	353.03	349.6A	376.12	378.74	420.87	402.20	373.03	363.04	358.27	354.22	351.59
1.00	351.35	353.03	349.6A	376.89	378.50	421.34	402.20	372.56	363.04	358.03	354.22	351.39
2.00	351.12	352.31	349.6A	376.12	378.50	421.81	402.20	372.56	362.80	358.03	354.46	351.35
3.00	351.83	352.55	349.6A	376.36	378.97	421.81	402.20	372.56	362.80	357.80	354.22	351.35
4.00	351.83	352.31	349.6A	376.60	379.21	421.58	401.73	373.03	362.56	357.80	354.22	351.35
5.00	351.83	353.50	349.6A	376.60	379.45	421.34	401.73	372.32	362.32	357.56	353.98	351.35
5.08	351.63	353.26	349.6A	376.60	379.45	421.58	401.73	372.32	362.32	357.80	353.98	351.35
5.17	351.83	353.50	349.6A	376.60	379.21	421.58	401.49	372.56	362.56	357.80	353.98	351.35
5.25	352.07	353.03	349.6A	376.36	378.97	421.11	401.49	372.56	362.32	357.80	353.98	351.35
5.33	351.83	352.79	349.6A	376.36	378.74	419.93	401.26	372.08	362.32	357.80	353.98	351.35
5.42	351.59	352.55	349.6A	376.12	378.50	419.22	401.02	372.32	362.32	357.80	353.98	351.35
5.50	351.35	353.03	349.6A	376.89	378.26	418.51	400.55	372.56	362.32	357.56	353.98	351.35
5.58	351.12	353.03	349.6A	376.89	378.26	417.56	400.31	371.84	362.32	357.56	353.98	351.35
5.67	351.12	352.79	349.6A	376.89	378.26	417.09	400.07	372.08	362.32	357.56	353.98	351.35
5.75	351.12	353.26	349.6A	376.65	378.02	416.38	399.84	372.08	362.32	357.56	353.98	351.35
5.83	351.12	353.50	349.6A	376.65	378.02	415.68	399.60	372.32	362.32	357.56	353.98	351.35
5.92	351.35	353.50	349.6A	376.65	378.02	414.97	399.36	372.08	362.09	357.56	353.98	351.35
6.00	351.35	353.50	349.6A	376.65	378.02	414.02	399.13	371.84	362.32	357.56	353.98	351.35
6.08	351.35	353.03	349.6A	376.65	378.02	413.79	398.89	371.84	362.09	357.56	353.98	351.35
6.17	351.35	353.26	349.6A	376.65	378.02	413.08	398.65	371.84	362.09	357.56	353.98	351.35
6.25	351.35	353.26	349.6A	376.65	378.02	412.84	398.42	372.08	362.09	357.56	353.98	351.35
6.33	351.59	353.50	349.6A	376.65	378.02	412.13	398.42	371.61	362.09	357.56	353.98	351.35
6.42	351.59	353.03	349.6A	376.65	378.02	411.66	398.18	372.08	362.09	357.56	353.98	351.35
6.50	351.59	352.55	349.6A	376.65	378.02	411.19	398.18	372.08	362.09	357.56	353.98	351.35
6.58	351.83	352.79	349.6A	376.65	378.02	411.19	398.18	371.84	362.09	357.56	353.98	351.35
6.67	351.83	352.79	349.6A	376.65	378.02	410.48	397.94	372.08	362.09	357.56	353.98	351.35
6.75	352.07	353.26	349.6A	376.65	378.02	410.24	397.94	372.08	362.09	357.56	353.98	351.35
6.83	351.59	353.26	349.6A	376.65	378.02	409.77	397.71	371.84	362.32	357.56	353.98	351.35
6.92	351.59	353.03	349.6A	376.65	378.02	409.53	397.71	372.08	362.32	357.56	353.98	351.35
7.00	351.59	353.74	349.6A	376.65	378.02	409.30	397.47	372.56	362.32	357.80	353.98	351.35
7.08	351.59	353.50	349.6A	376.65	378.02	409.06	397.47	372.32	362.56	357.80	353.98	351.35
7.17	351.59	353.26	349.6A	376.65	378.02	408.59	397.47	372.08	362.56	357.80	353.98	351.35
7.25	351.59	353.50	349.6A	376.65	378.02	408.12	397.23	372.32	362.56	357.80	353.98	351.35
7.33	351.59	353.03	349.6A	376.65	378.02	407.64	397.23	372.08	362.56	358.03	353.98	351.35
7.42	351.59	353.26	349.6A	376.65	378.02	407.64	397.23	372.08	362.56	358.03	353.98	351.35
7.50	351.59	353.50	349.6A	376.65	378.02	407.41	397.00	372.08	362.56	358.03	353.98	351.59
7.58	351.35	353.26	349.6A	376.65	377.79	407.17	397.00	372.56	362.80	358.03	354.22	351.35
7.67	351.12	353.74	349.6A	376.65	377.79	406.93	396.76	372.56	363.04	358.27	354.22	351.35
7.75	351.12	353.03	349.6A	376.65	377.79	406.70	396.76	372.32	363.04	358.27	354.22	351.35
7.83	351.35	353.74	349.6A	376.65	377.79	406.46	396.76	372.56	363.04	358.27	354.22	351.59
7.92	351.35	353.26	349.6A	376.65	377.79	406.46	396.76	372.80	363.04	358.51	354.22	351.59
8.00	351.59	352.79	349.6A	376.65	377.79	406.22	396.52	372.80	363.28	358.51	354.46	351.59
8.08	351.59	352.79	349.6A	376.65	377.79	405.75	396.52	372.32	363.28	358.51	354.22	351.59
8.17	351.59	353.50	349.6A	376.65	377.79	405.51	396.52	372.56	363.28	358.51	354.46	351.59
8.25	351.59	353.26	349.6A	376.65	377.79	405.28	396.52	372.56	363.28	358.51	354.46	351.59
8.33	351.35	353.03	349.6A	376.41	377.79	405.28	396.29	372.80	363.52	358.75	354.46	351.59
8.42	351.35	352.79	349.6A	376.41	377.79	405.28	396.29	372.56	363.52	358.75	354.46	351.59
8.50	351.35	353.03	349.6A	376.41	377.79	404.10	396.05	372.80	363.75	358.99	354.46	351.59
9.00	351.35	353.03	349.6A	375.17	377.55	403.15	395.81	373.51	364.23	359.23	355.17	351.83
10.00	351.35	352.79	349.6A	375.17	377.31	402.44	395.57	374.22	364.47	359.46	355.41	352.07
11.00	351.35	352.55	349.6A	375.17	377.31	402.20	395.57	374.22	364.71	359.46	355.41	352.07
12.00	351.59	352.79	349.6A	375.17	377.55	401.73	395.57	373.75	364.47	359.46	355.41	351.83
13.00	351.35	352.79	349.6A	375.41	377.55	401.73	395.57	373.75	364.47	359.46	355.41	351.83
14.00	351.12	352.55	349.6A	375.41	377.55	401.97	395.34	373.98	364.47	359.70	355.41	352.07
15.00	351.35	352.55	349.6A	375.41	377.79	401.97	395.34	373.98	364.47	359.46	355.41	352.07
16.00	351.59	352.79	349.6A	375.65	377.79	402.20	395.10	373.75	364.47	359.46	355.41	352.07
17.00	351.35	352.31	349.6A	375.65	378.02	402.20	394.86	373.98	364.47	359.46	355.17	352.07
18.00	351.59	352.55	349.6A	375.65	378.02	402.20	394.86	373.75	364.23	359.23	355.17	352.07
19.00	351.59	352.55	349.6A	375.65	378.02	402.20	394.86	374.22	364.23	359.23	355.17	352.07
20.00	351.35	352.79	349.6A	376.65	378.02	402.44	394.86	374.22	363.28	358.51	354.70	351.83
30.00	351.59	352.55	349.6A	376.84	379.45	405.28	394.39	372.80				

RUN 27A TIME (MIN)	PELLET									
	FATH1	RATH2	FILET	2	3	4	5	6	7	8
0	350.88	352.31	349.20	375.89	425.59	411.66	375.17	363.52	358.27	354.22
1.00	350.88	352.55	349.20	375.65	425.82	411.42	374.70	363.52	358.27	354.22
2.00	350.88	352.07	349.20	375.65	426.06	411.66	375.17	363.52	358.27	354.22
3.00	350.88	352.07	349.20	375.65	425.59	411.66	374.70	363.52	358.27	354.22
4.00	350.88	352.07	349.20	375.65	425.12	411.90	374.46	363.52	358.27	354.46
5.00	351.35	352.79	349.20	375.65	424.88	412.37	374.93	363.52	358.27	354.46
5.08	351.35	353.03	349.20	375.65	424.88	412.37	374.93	363.52	358.27	354.46
5.17	351.12	353.03	349.20	375.41	424.64	412.37	374.93	363.52	358.27	354.46
5.25	351.35	353.03	349.20	375.41	424.17	412.37	374.93	363.52	358.27	354.22
5.33	351.54	353.03	349.20	375.17	423.23	412.13	375.17	363.52	358.27	354.22
5.42	351.35	353.26	349.20	375.17	422.76	411.90	375.17	363.52	358.27	354.22
5.50	351.35	353.26	349.20	374.93	421.81	411.66	375.17	363.52	358.27	354.22
5.58	351.35	353.03	349.20	374.93	421.11	411.42	374.93	363.52	358.27	353.98
5.67	351.35	352.07	349.20	374.93	419.93	410.95	374.93	363.52	358.27	353.98
5.75	351.35	353.03	349.20	374.93	419.45	410.95	374.46	363.52	358.27	353.98
5.83	351.35	353.26	349.20	374.93	418.75	410.71	375.17	363.52	358.27	353.98
5.92	351.35	352.79	349.20	374.93	418.27	410.48	375.17	363.52	358.27	353.74
6.00	351.35	352.31	349.20	374.93	417.33	410.24	375.17	363.52	358.27	353.74
6.08	351.35	352.55	349.20	374.93	416.86	410.24	374.93	363.52	358.27	353.74
6.17	351.35	353.26	349.20	374.93	416.38	410.01	375.17	363.52	358.27	353.74
6.25	351.12	353.03	349.20	374.93	415.68	410.01	375.17	363.52	358.27	353.74
6.33	350.88	353.03	349.20	374.93	415.20	409.77	375.17	363.75	358.27	353.74
6.42	350.64	352.79	349.97	375.17	414.73	409.53	375.17	363.75	358.27	353.98
6.50	350.64	352.55	349.97	375.17	414.02	409.53	375.17	363.75	358.27	353.74
6.58	350.64	352.55	349.97	375.17	413.55	409.53	374.93	363.75	358.27	353.98
6.67	351.12	352.55	349.97	375.17	413.08	409.30	375.17	363.75	358.27	353.98
6.75	350.88	352.31	349.97	375.17	412.61	409.30	375.17	363.99	358.51	353.98
6.83	351.12	352.07	349.97	375.17	412.13	409.06	375.41	363.99	358.27	353.98
6.92	351.12	351.83	349.97	375.17	411.90	409.06	375.41	363.99	358.51	353.98
7.00	351.12	352.55	349.97	375.17	411.42	409.06	375.17	363.99	358.51	353.98
7.08	350.88	351.83	349.97	375.17	410.95	408.82	374.93	363.99	358.51	353.98
7.17	351.12	352.31	349.97	375.17	410.71	408.82	375.65	363.99	358.51	354.22
7.25	350.88	352.31	349.97	375.17	410.48	408.82	375.65	363.99	358.51	354.22
7.33	350.88	352.55	349.97	375.17	409.77	408.59	375.41	364.23	358.51	354.22
7.42	350.64	353.03	349.97	375.17	409.53	408.59	375.65	364.23	358.75	354.22
7.50	350.64	353.03	349.97	375.17	409.06	408.35	375.41	364.23	358.75	354.46
7.58	351.12	352.79	349.97	375.17	409.06	408.35	375.41	364.47	358.75	354.46
7.67	351.12	353.03	349.97	375.17	408.59	408.35	375.41	364.47	358.75	354.46
7.75	351.12	353.26	349.97	375.17	408.35	408.35	375.65	364.47	358.75	354.46
7.83	351.12	352.79	349.97	375.17	407.88	408.12	375.89	364.47	358.99	354.46
7.92	350.64	352.79	349.97	375.17	407.88	408.12	376.36	364.71	358.99	354.46
8.00	350.88	353.03	349.97	375.17	407.41	408.12	376.12	364.71	358.99	354.46
8.08	350.88	353.03	349.97	375.17	407.41	408.12	375.89	364.71	358.99	354.46
8.17	351.12	353.03	349.97	375.17	407.17	407.88	376.36	364.94	358.99	354.46
8.25	350.88	352.31	349.97	375.17	406.93	407.88	376.12	364.94	358.99	354.70
8.33	351.12	352.07	349.97	375.17	406.46	407.88	376.36	364.94	358.99	354.70
8.42	350.88	352.07	349.97	375.17	406.46	407.41	377.07	365.42	359.46	354.93
9.00	350.88	352.55	349.97	375.17	405.28	406.46	377.79	365.90	359.94	355.17
10.00	350.88	352.07	349.97	375.17	404.10	406.46	378.26	366.37	360.42	355.17
11.00	350.88	352.07	349.97	375.17	403.39	405.75	378.74	366.61	360.42	355.41
12.00	350.88	351.83	349.97	375.17	402.91	405.28	378.50	366.61	360.66	355.65
13.00	350.88	352.07	349.97	374.93	402.68	405.04	379.21	367.09	360.66	355.41
14.00	350.88	352.55	349.97	374.93	402.44	404.80	379.21	367.32	360.89	355.17
15.00	350.88	352.55	349.20	375.17	401.97	404.80	379.21	367.32	360.89	355.41
16.00	350.88	352.31	349.97	375.41	401.97	404.57	379.21	367.32	360.89	355.41
17.00	350.88	352.79	349.97	375.17	401.97	404.33	379.21	367.32	360.89	355.65
18.00	350.88	352.79	349.97	375.17	401.97	404.33	379.21	367.32	360.89	355.65
19.00	350.88	352.55	349.97	375.17	401.97	404.10	378.97	367.32	361.13	355.41
20.00	351.35	352.31	349.20	375.41	402.44	404.10	378.97	367.32	360.66	355.17
30.00	350.88	352.31	349.20	375.41	404.33	404.57	378.26	366.61		

RUN 27B									
TIME (MTH)									
0	1	2	3	4	5	6	7	8	9
1.00	351.59	341.11	418.98	397.71	371.84	362.56	357.80	353.9A	351.35
2.00	351.12	341.11	418.75	397.71	371.37	362.09	357.56	353.9A	351.35
3.00	351.59	341.11	419.22	397.71	370.89	361.85	357.56	353.9A	351.35
4.00	351.59	341.11	419.22	397.47	371.37	362.09	357.56	354.22	351.59
5.00	351.12	340.87	418.98	397.71	371.61	362.09	357.56	354.22	351.59
6.00	351.12	340.87	419.22	397.71	371.37	362.09	357.56	353.9A	351.59
7.00	351.35	340.87	419.22	397.71	371.37	362.09	357.56	353.9A	351.59
8.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
9.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
10.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
11.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
12.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
13.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
14.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
15.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
16.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
17.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
18.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
19.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
20.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59
30.00	351.35	340.87	419.22	397.71	371.13	362.09	357.56	353.9A	351.59

RUN 2HA													
TIME (MIN)													
U		BATH1	BATH2	INLET	PELLET	2	3	4	5	6	7	8	9
1.00		351.35	352.07	349.69	375.65	378.02	394.15	389.41	373.03	363.99	359.23	354.93	352.07
2.00		351.59	352.79	349.68	375.41	378.02	394.63	389.65	372.80	363.99	359.23	354.93	352.07
3.00		351.35	352.07	349.68	375.41	377.79	395.10	389.65	372.80	363.99	358.99	354.93	351.83
4.00		351.59	352.79	349.68	375.17	377.79	394.63	389.65	372.56	363.75	358.99	354.93	351.83
5.00		351.35	353.03	349.68	374.93	377.55	393.92	389.65	373.03	364.23	359.23	355.17	352.07
5.17		351.59	352.31	349.68	374.93	377.55	393.92	389.65	373.03	364.23	359.23	355.17	352.07
5.25		351.59	352.31	349.68	374.93	377.55	394.15	389.65	372.56	364.23	359.23	355.17	351.83
5.33		351.59	352.07	349.68	375.17	378.02	394.15	389.65	372.56	364.23	359.23	355.17	352.07
5.42		351.59	352.31	349.68	375.41	378.02	394.06	390.36	373.75	364.47	359.46	355.17	352.07
5.50		351.12	352.31	349.68	375.65	378.26	395.34	390.84	373.75	364.47	359.46	355.17	351.83
5.58		351.12	352.55	349.68	375.65	378.50	395.34	391.07	372.51	364.71	359.46	355.17	352.07
5.67		351.35	352.55	349.68	375.89	378.50	396.05	391.55	374.22	364.94	359.70	355.41	352.07
5.75		351.35	352.55	349.68	375.89	378.50	396.05	391.78	374.46	364.94	359.94	355.41	352.07
5.83		351.83	352.31	349.68	375.89	378.74	396.52	392.26	374.22	365.18	359.94	355.65	352.07
5.92		351.83	352.31	349.68	375.89	378.74	396.76	392.26	374.70	365.18	360.18	355.65	352.07
6.00		351.59	352.55	349.68	376.12	378.74	397.00	392.73	374.46	365.42	360.18	355.65	352.07
6.08		351.83	352.55	349.68	376.12	378.74	397.47	392.97	374.70	365.42	360.18	355.65	352.07
6.17		351.59	352.55	349.68	376.12	378.74	397.71	393.21	374.93	365.42	360.18	355.65	352.07
6.25		351.59	353.03	349.68	376.12	378.74	398.42	393.44	374.93	365.66	360.18	355.65	352.07
6.33		351.59	352.79	349.68	376.12	378.74	398.65	393.68	375.17	365.66	360.42	355.65	352.07
6.42		351.59	352.79	349.68	376.12	378.97	398.89	393.92	375.17	365.66	360.42	355.65	352.07
6.50		351.83	352.79	349.68	376.12	378.97	399.13	394.15	375.17	365.66	360.42	355.65	352.07
6.58		351.59	353.03	349.68	376.12	378.97	399.36	394.39	375.17	365.66	360.42	355.65	352.07
6.67		351.83	353.03	349.68	376.12	378.97	399.64	394.63	375.41	365.66	360.42	355.65	352.07
6.75		351.59	353.03	349.68	376.12	378.97	400.07	394.86	375.17	365.66	360.42	355.65	352.07
6.83		351.83	353.26	349.68	376.36	378.97	400.31	394.86	375.17	365.66	360.42	355.65	352.07
6.92		351.83	353.26	349.68	376.36	378.97	400.78	395.10	374.70	365.66	360.42	355.65	352.07
7.00		351.83	353.26	349.68	376.36	378.97	401.02	395.34	374.70	365.66	360.42	355.65	352.07
7.08		351.83	353.03	349.68	376.36	379.21	401.73	395.57	374.70	365.66	360.42	355.65	352.07
7.17		351.83	352.79	349.68	376.36	379.21	401.99	395.57	374.70	365.42	360.18	355.41	351.83
7.25		352.07	352.79	349.68	376.36	379.21	401.97	395.57	374.93	365.42	360.18	355.41	351.83
7.33		352.07	352.55	349.68	376.36	379.21	401.97	395.81	374.70	365.42	360.18	355.41	351.83
7.42		352.07	352.55	349.68	376.36	379.21	402.44	395.81	374.70	365.42	359.94	355.41	351.83
7.50		351.83	353.26	349.68	376.36	379.21	402.91	395.81	374.70	365.42	359.94	355.41	351.83
7.58		351.83	353.50	349.68	376.36	379.21	402.91	396.05	374.70	365.18	359.94	355.41	351.83
7.67		351.35	352.79	349.68	376.36	379.21	403.15	396.05	374.46	365.18	359.94	355.17	351.83
7.75		351.12	352.55	349.68	376.36	379.21	403.39	396.29	374.46	365.18	359.70	355.17	351.83
7.83		351.12	353.03	349.68	376.36	379.21	403.62	396.29	374.22	365.18	359.70	355.17	351.83
7.92		351.35	352.79	349.68	376.36	379.45	404.10	396.29	374.70	364.94	359.70	355.17	351.83
8.00		351.12	352.07	349.68	376.60	379.45	404.33	396.29	374.22	364.94	359.70	355.17	351.83
8.08		351.12	352.31	349.68	376.60	379.45	404.57	396.52	374.46	364.94	359.46	355.17	351.83
8.17		351.35	352.79	349.68	376.60	379.45	404.80	396.52	374.22	364.71	359.46	355.17	351.83
8.25		351.35	352.79	349.68	376.60	379.69	405.04	396.52	374.22	364.71	359.46	354.93	351.83
8.33		351.12	353.03	349.68	376.84	379.69	405.51	396.76	374.70	364.71	359.46	354.93	351.83
8.42		351.12	353.26	349.68	376.84	379.69	405.28	396.76	373.98	364.47	359.46	354.93	351.83
8.50		350.88	352.55	349.68	377.07	379.92	406.22	397.00	373.75	364.47	359.23	354.93	351.59
9.00		351.35	352.79	350.16	377.07	379.92	408.35	397.71	374.51	363.75	358.75	354.70	351.83
10.00		351.59	353.03	350.16	377.07	379.92	408.82	397.71	373.51	363.75	358.75	354.70	351.83
11.00		351.59	352.55	349.68	377.07	379.92	410.24	397.94	372.80	363.75	358.27	354.70	351.83
12.00		351.83	352.55	349.68	376.84	379.92	411.19	398.42	372.80	362.80	358.03	354.46	351.83
13.00		351.59	352.79	349.68	376.84	379.69	411.66	398.89	372.08	362.56	358.03	354.46	351.59
14.00		351.35	352.55	350.16	376.84	379.69	412.13	398.89	372.08	362.32	357.80	354.46	351.83
15.00		351.03	353.50	350.16	377.07	379.92	412.13	399.13	371.84	362.32	357.80	354.22	351.59
16.00		351.59	353.26	350.16	377.31	380.16	412.37	399.13	372.32	362.56	357.80	354.22	351.59
17.00		352.07	353.03	350.16	377.55	380.64	412.61	398.89	371.84	362.32	357.80	354.22	351.59
18.00		352.07	352.55	350.16	377.79	380.87	412.84	398.65	371.84	362.09	357.56	354.22	351.59
19.00		351.59	352.79	350.16	377.79	381.11	413.55	397.94	371.84	361.85	357.56	354.22	351.59
20.00		352.31	352.31	350.16	378.26	381.35	413.55	397.71	371.13	361.85	357.56	354.22	351.59
30.00		352.07	353.26	350.16	378.02	381.11	413.79	397.71	371.37	362.09	357.56	354.22	351.83

TIME (MIN)	PATH1	PATH2	TRIPLET	PELLET	2	3	4	5	6	7	8	9
348.25	348.97	348.97	346.34	350.42	361.61	362.56	362.09	362.56	365.42	367.32	363.04	355.11
348.25	349.44	349.44	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.04	355.17
348.01	349.20	349.20	346.34	360.66	361.95	362.80	362.09	362.80	365.18	367.32	363.04	355.17
348.01	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
347.77	348.97	348.97	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.41
347.77	348.97	348.97	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.41
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.01	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.25	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85	362.32	365.42	367.32	363.28	355.41
348.01	349.68	349.68	346.34	360.66	361.95	362.56	362.09	362.80	365.18	367.32	363.28	355.17
348.01	349.44	349.44	346.34	360.66	361.95	362.80	362.09	362.56	365.42	367.32	363.28	355.17
348.25	349.20	349.20	346.34	360.66	361.95	362.56	361.85					

TIME (MIN)	RAH1	RAH2	INLET	PELLET	2	3	4	5	6	7	8	9
0												
1.00	348.01	348.73	346.5A	362.56	363.99	365.70	365.66	364.71	362.32	359.23	354.22	349.6A
2.00	348.01	348.97	346.5A	362.56	363.99	365.90	365.66	364.23	362.32	359.23	354.22	349.68
3.00	347.77	349.20	346.5A	362.56	363.99	366.13	365.66	364.47	362.32	359.46	354.46	349.92
4.00	348.01	348.97	346.5A	362.80	363.99	366.13	365.42	364.47	362.32	359.23	354.46	349.6A
5.00	348.01	348.97	346.5A	362.80	363.99	366.13	365.66	364.23	362.32	359.23	354.22	349.6A
5.0A	348.25	348.97	346.5A	362.80	363.99	366.61	365.66	364.47	362.09	359.23	354.46	349.6A
5.17	348.49	348.97	346.5A	362.80	363.99	366.37	365.66	364.47	362.09	359.23	354.46	349.6A
5.25	348.25	348.97	346.5A	362.56	363.99	366.85	365.90	364.94	362.56	359.46	354.70	349.92
5.33	348.49	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
5.42	348.49	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
5.50	348.49	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
5.5A	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
5.67	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
5.75	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
5.83	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
5.92	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.09	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.17	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.25	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.33	348.49	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.42	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.50	348.49	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.5A	348.49	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.67	348.49	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.75	348.49	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.83	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
6.92	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.0A	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.17	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.25	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.33	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.42	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.50	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.5A	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.67	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.75	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.83	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
7.92	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
8.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
8.0A	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
8.17	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
8.25	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
8.33	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
8.42	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
9.00	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
10.00	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
11.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
12.00	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
13.00	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
14.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
15.00	348.01	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
16.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
17.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
18.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
19.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
20.00	348.25	348.97	346.5A	362.80	364.23	366.85	365.90	364.94	362.56	359.46	354.70	349.92
30.00	348.73	350.40	346.82	361.85	363.04	364.47	363.52	363.75	366.37	368.28	363.52	355.65

TIME (MIN)	BATH1	RATH2	INLET	PELLET	2	3	4	5	6	7	8	9
0	348.01	349.48	346.34	361.61	362.80	364.23	363.28	364.23	366.13	367.32	362.56	354.46
1.00	348.25	349.20	346.34	361.37	362.56	364.23	363.28	363.52	366.37	367.32	362.56	354.46
2.00	348.01	349.44	346.34	361.61	362.80	363.99	363.28	363.75	366.37	367.32	362.56	354.46
3.00	348.01	349.48	346.34	361.61	362.80	363.99	363.28	363.52	366.13	367.32	362.56	354.46
4.00	348.01	349.44	346.34	361.61	362.80	364.23	363.04	363.28	366.13	367.32	362.56	354.46
5.00	348.01	349.20	346.34	361.37	362.80	363.99	363.28	363.52	366.13	367.32	362.56	354.46
5.0A	348.25	349.44	346.34	361.61	362.80	364.23	363.04	363.28	366.13	367.32	362.56	354.46
5.17	348.25	349.97	346.58	361.61	362.90	364.23	363.28	363.75	366.13	367.32	362.56	354.46
5.25	348.01	349.20	346.58	361.61	363.04	364.23	363.28	363.99	366.61	367.56	362.80	354.46
5.33	348.25	349.20	346.58	361.61	363.04	364.47	363.52	363.52	366.85	367.80	362.80	354.46
5.42	348.25	348.97	346.58	361.61	363.28	364.23	363.52	363.52	367.09	368.04	363.04	354.46
5.50	348.25	348.97	346.58	361.85	363.28	364.47	363.52	363.52	367.09	368.28	363.28	354.46
5.5A	348.25	349.20	346.58	361.85	363.28	364.47	363.52	363.52	367.32	368.51	363.52	354.46
5.67	348.01	349.20	346.58	362.09	363.28	364.47	363.52	363.75	367.32	368.75	363.52	354.46
5.75	348.25	349.20	346.58	362.09	363.28	364.71	363.52	364.23	367.32	368.99	363.99	354.46
5.83	348.25	349.20	346.58	362.09	363.28	364.47	363.52	364.23	367.56	368.99	363.99	354.46
5.92	348.25	348.97	346.58	362.09	363.28	364.47	363.52	364.23	367.56	369.23	364.23	354.46
6.00	348.25	348.97	346.58	362.09	363.28	364.47	363.52	363.52	367.56	369.47	364.47	354.46
6.0A	348.25	349.20	346.58	362.09	363.28	364.23	363.52	363.52	367.56	369.47	364.71	354.46
6.17	348.25	349.44	346.58	362.09	363.28	364.47	363.52	364.23	367.56	369.47	364.71	354.46
6.25	348.25	349.20	346.58	361.85	363.28	364.47	363.52	363.99	367.56	369.70	364.71	354.46
6.33	348.25	349.44	346.58	361.85	363.28	364.47	363.52	363.99	367.56	369.70	364.71	354.46
6.42	348.25	349.20	346.58	361.85	363.28	364.47	363.52	363.99	367.56	369.70	364.71	354.46
6.50	348.25	349.20	346.58	361.85	363.28	364.47	363.52	363.99	367.56	369.70	364.71	354.46
6.5A	348.01	349.20	346.58	361.85	363.28	364.47	363.52	363.99	367.56	369.70	364.71	354.46
6.67	348.25	349.02	346.58	361.85	363.28	364.47	363.52	363.99	367.56	369.70	364.71	354.46
6.75	348.25	349.44	346.58	361.85	363.28	364.47	363.52	363.99	367.56	369.70	364.71	354.46
6.83	348.25	349.44	346.58	361.85	363.28	364.47	363.52	363.99	367.56	369.70	364.71	354.46
6.92	348.25	349.44	346.34	361.85	363.28	364.23	363.04	363.75	367.32	370.18	365.42	355.89
7.00	348.25	349.44	346.34	361.85	363.28	364.23	363.04	363.75	367.32	370.18	365.42	355.89
7.0A	348.25	349.68	346.58	361.85	363.04	364.23	363.04	363.75	367.32	370.18	365.42	355.89
7.17	348.01	349.92	346.58	361.85	363.04	364.23	363.04	363.75	367.32	370.18	365.42	355.89
7.25	348.25	349.68	346.58	361.85	363.28	364.23	363.04	363.52	367.32	370.42	365.66	356.13
7.33	348.25	349.44	346.58	361.85	363.04	363.99	363.04	363.28	367.32	370.42	365.66	356.37
7.42	348.01	349.44	346.58	361.85	363.04	363.99	363.04	363.75	367.32	370.42	365.90	356.37
7.50	348.25	349.44	346.58	361.85	363.04	363.99	362.80	363.52	367.09	370.42	365.66	356.37
7.5A	348.25	349.68	346.58	361.85	363.04	363.99	362.80	363.52	367.32	370.42	365.90	356.37
7.67	348.49	349.44	346.58	361.85	363.04	363.75	362.80	363.28	367.32	370.42	365.66	356.37
7.75	348.25	349.44	346.58	361.61	363.04	363.99	362.80	363.28	367.32	370.42	365.90	356.37
7.83	348.49	349.68	346.58	361.61	363.04	363.75	362.80	363.52	367.09	370.42	365.90	356.37
7.92	348.25	349.44	346.58	361.85	363.04	363.75	362.80	363.04	367.09	370.42	365.66	356.37
8.00	347.77	349.20	346.58	361.61	363.04	363.75	362.56	363.28	367.09	370.42	365.90	356.37
8.0A	347.77	349.20	346.58	361.61	363.04	363.75	362.56	363.28	367.09	370.66	365.90	356.160
8.17	348.01	349.44	346.58	361.61	363.04	363.75	362.56	363.04	367.09	370.66	365.90	356.37
8.25	348.01	349.44	346.58	361.61	363.04	363.75	362.56	363.04	367.09	370.66	365.90	356.60
8.33	348.25	349.44	346.58	361.61	363.04	363.52	362.56	363.28	367.09	370.66	365.13	356.84
9.00	348.01	349.44	346.34	361.61	362.80	363.28	362.32	362.56	366.37	370.42	366.41	356.84
10.00	348.01	349.20	346.34	361.37	362.56	363.28	362.32	362.56	366.13	370.18	366.61	357.08
11.00	348.01	349.20	346.34	361.13	362.32	363.04	362.09	362.80	366.13	369.94	366.61	357.08
12.00	348.01	349.20	346.34	361.13	362.32	363.04	362.09	362.56	365.90	369.94	366.61	357.08
13.00	348.01	348.97	346.34	361.13	362.32	363.04	361.85	362.32	365.90	369.70	366.37	357.08
14.00	348.01	348.97	346.34	360.89	362.32	363.04	361.85	362.32	365.90	369.70	366.61	357.08
15.00	348.01	348.97	346.34	360.89	362.09	362.80	361.85	362.09	365.90	369.70	366.37	357.08
16.00	347.53	349.20	346.34	360.89	362.09	362.80	361.85	362.09	365.66	369.70	366.37	357.08
17.00	347.77	348.97	346.34	360.89	362.09	362.56	361.61	362.56	365.90	369.70	366.37	357.08
18.00	347.77	348.97	346.34	360.89	362.09	362.56	361.61	362.56	365.90	369.70	366.37	357.08
19.00	347.77	348.97	346.34	360.89	362.09	362.56	361.85	362.56	366.13	369.70	366.37	357.08
20.00	347.77	349.20	346.34	360.89	362.09	362.56	361.85	362.32	366.13	369.70	366.37	357.08
30.00	348.25	349.44	346.58	361.61	362.80	363.52	362.32	362.09	365.66	369.94	366.37	356.84

RUN 29D									
TIME (MIN)									
0									
1.00	RATH	RATH2	TILFT	PELLET	2	3	4	5	6
2.00	348.01	349.68	346.5A	361.13	362.56	362.80	361.85	362.56	364.37
3.00	348.01	349.44	346.5A	361.13	362.32	363.04	361.85	362.80	366.37
4.00	348.01	349.68	346.5A	361.13	362.32	362.80	362.09	362.80	366.37
5.00	348.25	349.44	346.5A	361.13	362.32	362.80	361.85	362.56	366.37
5.08	348.01	349.92	346.5A	361.13	362.32	362.80	361.85	362.56	366.37
5.17	348.01	349.92	346.5A	361.13	362.32	362.80	361.85	362.32	366.37
5.25	348.25	349.20	346.34	360.89	362.32	363.04	361.85	362.32	366.13
5.33	348.25	349.20	346.34	360.89	362.09	362.32	361.61	361.85	366.13
5.42	348.25	349.20	346.34	360.89	362.09	362.56	361.61	362.32	366.90
5.50	348.25	349.20	346.34	360.66	361.85	362.56	361.61	362.32	366.66
5.58	348.25	349.20	346.34	360.66	361.85	362.56	361.61	362.32	366.66
5.67	348.25	349.20	346.34	360.66	361.85	362.80	361.61	361.85	366.61
5.75	348.01	349.97	346.34	360.66	361.85	362.56	361.61	362.32	366.37
5.83	348.01	349.20	346.5A	360.66	361.85	362.80	361.61	362.32	366.37
5.92	348.01	349.20	346.34	360.66	361.85	363.04	361.61	362.32	366.13
6.00	348.01	349.20	346.34	360.66	361.85	362.56	361.61	362.32	366.90
6.08	348.01	349.44	346.34	360.66	361.85	362.56	361.61	362.09	366.66
6.17	348.25	349.44	346.34	360.66	361.85	362.80	361.85	362.56	366.66
6.25	348.25	349.20	346.34	360.66	362.09	362.80	361.85	362.56	366.66
6.33	348.25	349.44	346.34	360.66	362.09	362.80	361.85	362.56	366.61
6.42	348.25	349.20	346.34	360.66	362.09	362.80	361.61	362.09	366.42
6.50	348.01	349.44	346.34	360.66	362.09	362.56	361.85	362.56	366.42
6.58	347.77	349.68	346.34	360.66	362.09	362.80	361.85	362.56	366.42
6.67	347.77	349.20	346.34	360.66	362.09	362.80	361.85	362.56	366.42
6.75	347.77	349.20	346.34	360.89	362.09	363.04	361.85	362.80	366.42
6.83	347.77	349.44	346.34	360.89	362.09	362.56	361.85	362.56	366.42
6.92	347.77	349.44	346.34	360.89	362.09	362.56	361.85	362.32	366.42
7.00	348.01	349.20	346.34	360.89	362.09	362.80	361.85	362.56	366.42
7.08	348.01	348.97	346.34	360.89	362.09	362.80	361.85	362.56	366.42
7.17	348.25	348.97	346.34	360.89	362.09	363.04	361.85	362.56	366.42
7.25	348.25	348.97	346.34	360.89	362.09	363.04	361.85	362.56	366.42
7.33	348.25	348.97	346.34	360.89	362.09	362.80	361.85	362.56	366.42
7.42	348.25	348.97	346.34	360.89	362.09	362.80	361.85	362.56	366.42
7.50	348.01	348.97	346.34	360.89	362.09	363.04	361.85	362.80	366.42
7.58	348.01	348.97	346.34	360.89	362.09	363.04	361.85	362.56	366.42
7.67	348.25	348.97	346.34	360.89	362.09	363.04	362.09	362.80	366.42
7.75	348.01	348.97	346.34	360.89	362.09	363.04	362.09	362.56	366.42
7.83	348.01	349.44	346.34	360.89	362.09	362.80	362.09	362.56	366.42
7.92	348.01	349.20	346.34	360.89	362.09	363.04	362.09	363.04	366.42
8.00	348.25	349.44	346.34	360.89	362.09	363.04	362.09	362.56	366.42
8.08	348.01	349.20	346.34	360.89	362.09	363.04	362.09	362.56	366.42
8.17	348.01	348.97	346.34	360.89	362.09	363.04	362.09	362.56	366.42
8.25	348.01	348.97	346.34	360.89	362.09	363.04	362.09	362.56	366.42
8.33	348.01	348.97	346.34	361.13	362.32	363.28	362.32	363.04	366.42
9.00	348.25	349.20	346.34	361.13	362.32	363.52	362.32	363.28	366.42
10.00	347.77	348.97	346.34	361.13	362.32	363.52	362.32	363.28	366.42
11.00	348.01	348.97	346.34	361.13	362.32	363.52	362.32	363.28	366.42
12.00	348.25	349.20	346.34	361.13	362.32	363.52	362.32	363.28	366.42
13.00	347.77	349.20	346.34	361.13	362.32	363.52	362.32	363.28	366.42
14.00	348.01	349.44	346.34	361.13	362.32	363.52	362.32	363.28	366.42
15.00	348.25	349.44	346.34	361.13	362.32	363.52	362.32	363.28	366.42
16.00	348.01	349.68	346.5A	361.13	362.32	363.52	362.32	363.28	366.42
17.00	348.01	348.97	346.34	361.13	362.32	363.52	362.32	363.28	366.42
18.00	347.77	348.97	346.34	361.13	362.32	363.52	362.32	363.28	366.42
19.00	348.01	349.68	346.34	361.13	362.32	363.52	362.32	363.28	366.42
20.00	347.77	349.20	346.34	361.13	362.32	363.52	362.32	363.28	366.42
30.00	348.01	349.44	346.34	361.13	362.32	363.52	362.32	363.28	366.42

RUN 30A	BATH1	BATH2	INLET	PELLET	2	3	4	5	6	7	8	9
TIME (MIN)												
0	353.26	354.70	351.59	37A.26	3A1.11	401.73	394.39	373.9A	364.94	360.42	356.60	352.74
1.00	353.74	354.46	351.83	37A.26	3A1.11	401.73	394.63	373.9A	364.94	360.1A	356.37	352.50
2.00	353.50	354.46	351.59	37A.50	3A1.11	402.20	394.63	374.46	364.94	360.42	356.60	352.74
3.00	353.26	354.46	351.59	37A.26	3A1.11	401.97	394.86	373.9A	364.94	360.1A	356.37	352.50
4.00	353.74	354.70	351.59	37A.50	3A1.11	402.20	394.86	374.22	364.71	360.1A	356.37	352.50
5.00	353.74	354.22	351.83	37A.50	3A1.11	402.20	394.86	373.9A	364.71	360.1A	356.37	352.50
5.17	353.9A	354.70	351.59	37A.50	3A1.11	402.20	394.86	373.9A	364.71	360.1A	356.37	352.50
5.25	353.50	354.70	351.59	37A.26	3A1.11	403.15	395.57	374.70	364.94	360.42	356.60	352.74
5.33	353.03	354.70	351.59	37A.50	3A1.11	402.6A	395.34	374.70	364.94	360.42	356.60	352.74
5.42	353.74	354.46	351.59	37A.26	3A1.11	401.97	394.63	374.22	364.94	360.42	356.37	352.74
5.50	353.74	354.22	351.59	37A.26	3A1.11	401.97	394.39	374.22	364.71	360.42	356.37	352.74
5.58	353.9A	354.93	351.59	37A.26	3A1.11	401.26	393.92	373.9A	364.47	360.1A	356.37	352.50
5.67	353.74	354.46	351.83	37A.26	3A1.11	401.02	393.44	373.75	364.47	360.1A	356.37	352.50
5.75	353.74	354.70	351.83	37A.26	3A1.11	400.31	392.97	373.51	364.23	359.94	356.13	352.50
5.83	353.26	354.46	351.83	37A.26	3A1.11	400.07	392.73	372.80	363.99	359.70	356.13	352.50
5.92	353.74	354.46	351.83	37A.26	3A1.11	399.84	392.26	372.80	363.75	359.70	356.13	352.50
6.00	353.74	354.46	351.83	37A.26	3A1.11	399.60	392.02	372.80	363.75	359.70	356.13	352.50
6.08	353.74	354.46	351.83	37A.26	3A1.11	399.13	391.55	372.0A	363.52	359.46	355.89	352.50
6.17	353.74	354.70	351.83	37A.26	3A1.11	399.13	391.31	372.32	363.52	359.46	356.13	352.50
6.25	353.50	354.46	351.83	37A.26	3A1.11	398.65	391.07	372.08	363.2A	359.23	355.89	352.50
6.33	353.26	354.70	351.83	37A.26	3A1.11	398.18	390.84	371.61	363.2A	359.23	355.65	352.50
6.42	353.03	354.22	351.83	37A.26	3A1.11	398.1A	390.36	371.84	363.04	358.99	355.89	352.50
6.50	353.50	354.70	351.83	37A.26	3A1.11	398.1A	390.36	371.61	363.04	358.99	355.65	352.50
6.58	353.26	354.70	351.83	37A.26	3A1.11	397.94	390.12	371.61	362.80	358.99	355.65	352.50
6.67	353.03	354.22	351.83	37A.50	3A1.11	397.94	389.89	371.37	362.80	358.99	355.89	352.50
6.75	353.50	354.46	351.59	37A.50	3A1.11	397.23	389.65	370.89	362.80	358.99	355.65	352.50
6.83	353.74	354.70	351.59	37A.50	3A1.11	397.47	389.65	371.13	362.80	358.99	355.89	352.50
6.92	353.74	354.46	351.59	37A.74	3A1.11	397.23	389.41	371.13	362.80	358.99	355.65	352.50
7.00	353.50	354.46	351.59	37A.74	3A1.11	397.47	389.18	371.61	362.56	358.99	355.89	352.50
7.08	353.74	354.46	351.59	37A.74	3A1.59	397.00	389.18	371.13	362.56	358.75	355.89	352.50
7.17	353.74	354.46	351.59	37A.97	3A1.59	397.00	389.18	370.66	362.80	358.75	355.65	352.50
7.25	353.74	354.70	351.59	37A.97	3A1.59	397.00	388.94	371.37	362.56	358.75	355.89	352.50
7.33	353.74	354.46	351.59	37A.74	3A1.59	396.76	388.94	370.66	362.56	358.75	355.65	352.50
7.42	353.26	354.93	351.59	37A.74	3A1.82	396.52	388.70	370.66	362.56	358.75	355.65	352.50
7.50	353.50	354.93	351.83	37A.97	3A1.82	396.52	388.70	370.89	362.56	358.75	355.65	352.50
7.58	353.74	354.70	351.83	37A.97	3A1.82	396.52	388.47	370.89	362.56	358.75	355.65	352.50
7.67	353.74	354.93	351.83	37A.97	3A1.82	396.52	388.47	370.89	362.56	358.75	355.65	352.50
7.75	353.74	354.93	351.83	37A.97	3A2.06	396.52	388.47	371.13	362.80	358.75	355.65	352.50
7.83	353.74	354.46	351.59	37A.97	3A2.06	396.52	388.23	371.13	362.56	358.75	355.65	352.50
7.92	353.74	354.46	351.83	37A.21	3A2.06	396.52	387.99	370.89	362.56	358.75	355.65	352.50
8.00	353.74	354.93	351.83	37A.21	3A2.06	396.52	387.99	371.13	362.56	358.75	355.65	352.50
8.08	353.74	354.22	351.83	37A.21	3A2.1A	396.52	387.99	370.66	362.56	358.75	355.65	352.50
8.17	353.26	354.70	351.83	37A.21	3A2.1A	396.52	387.99	370.66	362.56	358.75	355.65	352.50
8.25	353.50	354.46	351.83	37A.21	3A2.30	396.52	387.99	370.89	362.80	358.75	355.65	352.50
8.33	353.50	354.46	351.83	37A.45	3A2.30	396.29	387.75	371.13	362.80	358.75	355.65	352.50
8.42	353.74	354.70	351.83	37A.45	3A2.30	396.29	387.75	371.13	362.80	358.75	355.65	352.50
9.00	353.50	354.46	351.83	37A.69	3A2.77	396.29	387.28	370.89	362.80	358.75	355.65	352.50
10.00	353.74	354.22	351.83	380.16	3A3.4A	396.52	386.81	370.66	362.56	358.75	355.65	353.03
11.00	353.50	354.93	351.59	380.64	3A3.72	396.52	386.33	369.94	362.56	358.75	355.65	353.26
12.00	353.26	354.70	351.83	380.87	3A3.96	397.23	386.33	370.1A	361.85	358.51	355.65	353.74
13.00	353.50	354.46	351.59	380.64	3A3.96	397.71	386.33	369.94	361.85	358.27	355.41	353.50
14.00	353.74	354.22	351.83	380.64	3A3.96	397.94	386.33	369.94	361.85	358.27	355.41	353.74
15.00	353.03	354.46	351.83	380.64	3A3.96	397.71	386.33	369.94	361.85	358.27	355.41	353.03
16.00	353.74	354.46	351.59	380.64	3A3.4A	397.94	386.33	369.94	361.85	358.51	355.41	353.74
17.00	353.50	354.22	351.83	380.40	3A3.72	398.18	386.33	370.1A	361.85	358.27	355.41	353.50
18.00	353.74	354.46	351.83	380.64	3A3.72	397.94	386.33	369.94	361.85	358.27	355.41	353.74
19.00	353.50	354.22	351.83	380.40	3A3.72	397.94	386.33	369.94	361.85	358.27	355.41	353.50
20.00	353.03	354.46	351.83	380.40	3A3.4A	397.94	386.33	369.94	361.85	358.27	355.41	353.03
30.00	353.74	354.22	351.59	380.16	3A3.25	397.47	386.33	369.94	361.85	358.27	355.17	353.03

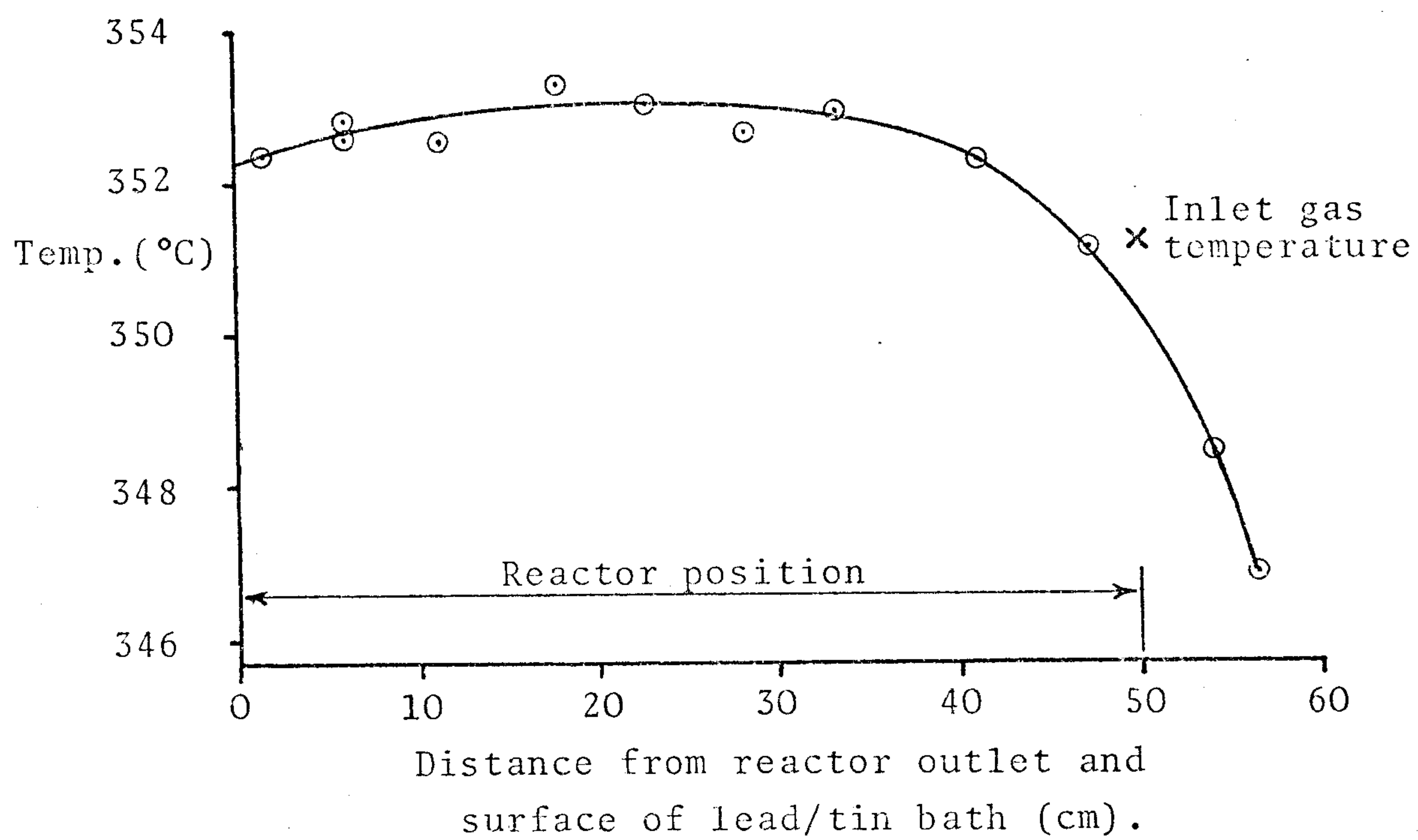
RUN 308										
TIME (MIN)										
0	RATH1	BATH2	INLET	PELLET	2	3	4	5	6	7
1.00	353.74	354.22	352.07	381.59	384.67	398.18	386.09	369.70	361.61	358.27
2.00	353.74	354.70	351.83	381.59	384.91	397.94	385.86	369.70	361.85	358.27
3.00	353.74	354.46	352.07	381.82	385.15	398.18	386.09	369.47	361.85	358.03
4.00	353.74	354.93	351.83	381.82	385.15	398.18	386.09	369.70	361.85	358.27
5.00	353.98	354.70	351.83	381.82	385.38	397.94	386.09	369.23	361.85	358.27
5.17	353.98	354.93	351.83	382.06	385.38	398.18	385.86	369.99	361.61	358.03
5.25	353.98	354.70	351.83	382.06	385.38	398.42	385.86	369.99	361.61	358.27
5.33	353.98	354.46	351.83	382.06	385.38	398.42	385.86	369.75	361.61	358.03
5.42	353.50	354.70	352.07	381.82	385.15	398.42	385.62	369.23	361.61	358.03
5.50	353.50	354.46	351.83	382.06	385.62	398.42	385.62	369.75	361.61	358.03
5.58	353.74	354.46	351.83	382.06	385.62	398.42	385.86	369.75	361.61	358.03
5.67	353.74	354.46	351.83	382.30	386.09	399.60	386.09	369.23	361.61	358.27
5.75	353.74	354.22	351.83	382.30	386.09	399.60	386.57	369.70	361.85	358.27
5.83	353.26	354.22	351.83	382.53	386.09	400.31	387.04	369.70	362.09	358.41
5.92	353.03	354.22	352.07	382.53	386.09	400.31	387.04	369.70	362.32	358.51
6.00	353.26	354.46	352.07	382.53	386.33	401.02	387.28	369.70	362.32	358.51
6.08	353.03	354.46	351.83	382.53	386.33	401.26	387.52	369.94	362.56	358.75
6.17	353.74	354.22	351.83	382.77	386.33	401.73	387.99	370.66	362.80	358.75
6.25	353.74	354.46	351.83	382.77	386.33	401.73	387.99	370.66	362.80	358.99
6.33	353.98	354.70	351.83	382.77	386.33	402.44	388.47	370.89	363.04	358.99
6.42	353.98	354.70	352.07	382.77	386.33	402.44	388.47	370.89	363.04	358.99
6.50	353.50	354.70	352.07	382.77	386.33	402.91	388.70	370.66	363.04	358.99
6.58	353.50	354.46	352.07	382.77	386.33	403.39	388.94	371.13	363.04	359.23
6.67	353.26	354.46	352.07	382.77	386.33	403.39	389.18	371.37	363.28	359.23
6.75	353.03	354.46	352.07	382.77	386.57	403.62	389.18	370.89	363.28	359.23
6.83	353.26	354.70	352.07	382.77	386.33	403.86	389.41	370.89	363.28	359.23
6.92	353.26	354.46	352.07	382.77	386.33	403.86	389.41	370.89	363.28	359.23
7.00	353.50	355.65	352.07	382.77	386.33	404.10	389.65	371.37	363.28	359.23
7.08	353.74	354.70	352.07	382.77	386.33	404.57	389.89	371.37	363.52	359.23
7.17	353.98	355.41	352.07	382.53	386.33	404.80	390.12	371.13	363.28	359.23
7.25	353.98	355.17	352.07	382.53	386.33	404.80	390.12	371.13	363.28	359.23
7.33	353.98	355.17	352.07	382.53	386.09	404.80	390.12	371.13	363.28	359.23
7.42	353.98	354.70	351.83	382.53	386.09	405.04	390.12	371.61	363.28	359.46
7.50	353.74	354.70	351.83	382.53	386.09	405.51	390.36	371.37	363.52	359.46
7.58	353.74	354.70	351.83	382.30	386.09	405.28	390.60	371.61	363.52	359.46
7.67	353.50	354.46	351.83	382.30	385.86	405.51	390.60	371.37	363.28	359.46
7.75	353.50	354.93	351.83	382.30	385.86	405.75	390.60	371.61	363.52	359.46
7.83	353.50	355.17	351.83	382.30	385.86	405.75	390.60	371.84	363.28	359.46
7.92	353.98	355.17	351.83	382.30	385.86	406.22	391.07	371.84	363.52	359.46
8.00	353.98	354.93	351.83	382.06	385.62	406.22	391.07	371.61	363.52	359.23
8.08	353.74	355.41	351.83	382.06	385.62	405.99	391.07	371.61	363.28	359.23
8.17	354.46	354.70	351.83	381.82	385.62	406.22	391.31	372.08	363.28	359.23
8.25	354.22	355.17	351.83	381.82	385.38	406.22	391.31	371.84	363.28	359.23
8.33	354.22	355.17	351.83	381.82	385.38	406.22	391.55	371.37	363.28	359.23
8.42	354.22	355.41	351.83	381.59	385.38	406.70	391.55	371.84	363.28	359.23
8.50	353.03	355.41	351.83	381.59	385.15	406.70	391.78	371.84	363.28	359.23
9.00	353.74	355.41	351.83	381.59	384.67	407.17	392.02	371.84	363.52	359.46
10.00	353.03	354.93	351.83	380.64	384.20	407.17	392.73	371.61	363.75	359.46
11.00	353.74	354.70	351.83	380.16	383.48	406.70	393.44	372.32	363.75	359.46
12.00	353.74	354.46	351.83	380.16	383.48	406.22	393.92	372.32	363.52	359.46
13.00	353.98	354.46	351.83	380.16	383.48	405.99	394.39	372.56	363.52	359.46
14.00	353.98	354.70	351.83	380.40	383.72	405.75	393.92	372.56	363.52	359.46
15.00	353.50	354.70	352.07	380.87	384.20	405.75	393.68	372.08	363.52	359.23
16.00	353.74	354.70	351.83	381.11	384.67	406.22	393.68	372.80	363.75	359.46
17.00	353.50	354.22	351.83	381.11	384.43	405.75	393.68	372.08	363.52	359.46
18.00	353.74	355.17	351.83	380.87	384.20	405.75	393.44	372.56	363.52	359.46
19.00	353.74	354.46	351.83	380.64	383.96	406.22	393.44	373.03	363.99	359.46
20.00	353.26	354.46	351.83	380.64	383.96	406.22	393.68	372.32	363.75	359.46
30.00	353.74	355.17	351.83	381.11	384.43	405.75	393.21	371.84	363.52	359.46

RUN	TIME (MIN)	RATH1	RATH2	INLET	FELETT	2	3	4	5	6	7	A	9
0		153.74	154.70	152.07	180.40	383.48	404.80	393.68	373.03	364.23	359.94	356.37	351.74
1.00		154.22	154.70	152.07	180.16	383.48	404.57	393.68	373.03	364.23	359.94	356.60	351.74
2.00		154.98	154.70	152.07	180.40	383.48	404.33	393.92	373.03	363.99	359.94	356.37	351.98
3.00		154.98	154.93	152.07	180.40	383.72	404.33	393.68	373.03	363.99	359.70	356.37	351.98
4.00		154.50	154.70	152.07	180.40	383.72	404.33	393.68	373.03	363.99	359.70	356.13	351.74
5.00		154.50	154.46	152.07	180.64	383.96	404.57	393.44	373.56	363.99	359.70	356.13	351.74
5.17		154.74	154.46	152.07	180.64	383.96	404.57	393.44	373.56	364.23	359.70	356.13	351.74
5.25		154.98	154.46	152.07	180.64	383.96	404.57	393.44	373.80	364.23	359.70	356.13	351.74
5.33		154.74	154.46	152.07	180.64	384.20	404.80	393.44	373.03	364.23	359.70	356.13	351.50
5.42		154.50	154.70	152.31	180.87	384.43	405.28	393.44	373.27	364.23	359.70	356.13	351.74
5.50		154.26	154.70	152.31	181.35	384.41	406.22	393.92	373.27	364.23	359.70	356.13	351.74
5.58		154.50	154.70	152.31	181.35	385.15	406.22	394.39	373.75	364.47	359.94	356.37	351.74
5.67		154.26	154.70	152.31	181.92	385.38	407.64	394.86	373.98	364.71	359.94	356.37	351.74
5.75		154.50	154.93	152.31	181.82	385.42	408.12	395.34	373.98	364.94	359.94	356.37	351.74
5.83		154.26	154.93	152.31	182.06	385.46	408.82	395.57	374.22	364.94	359.94	356.37	351.74
5.92		154.50	155.17	152.31	182.30	385.46	409.30	396.05	374.22	364.94	360.18	356.37	351.74
6.00		154.74	154.70	152.31	182.30	386.09	410.24	396.29	374.46	365.18	360.18	356.60	351.74
6.08		154.98	154.93	152.31	182.30	386.09	410.48	396.52	374.46	365.42	360.42	356.60	351.74
6.17		154.74	155.17	152.31	182.53	386.33	411.19	397.00	374.46	365.42	360.42	356.60	351.74
6.25		154.74	154.93	152.31	182.53	386.33	411.90	397.00	374.70	365.42	360.42	356.60	351.74
6.33		154.50	154.93	152.31	182.53	386.33	412.37	397.47	374.93	365.42	360.42	356.60	351.74
6.42		154.50	154.93	152.31	182.53	386.33	412.84	397.47	374.93	365.42	360.42	356.60	351.74
6.50		154.50	154.70	152.31	182.77	386.57	413.31	397.71	374.93	365.42	360.42	356.60	351.74
6.58		154.50	154.70	152.31	182.77	386.57	413.79	397.94	374.93	365.42	360.42	356.60	351.74
6.67		154.74	154.93	152.31	182.77	386.57	414.26	397.94	374.70	365.42	360.42	356.60	351.74
6.75		154.50	154.70	152.31	182.77	386.57	414.73	397.94	374.70	365.42	360.42	356.60	351.74
6.83		154.74	154.93	152.31	182.77	386.81	415.44	398.18	374.70	365.42	360.42	356.60	351.98
6.92		154.98	154.93	152.31	182.77	386.81	415.68	398.18	374.70	365.42	360.42	356.60	351.98
7.00		154.74	155.17	152.31	182.77	386.81	416.15	398.42	374.70	365.42	360.42	356.60	351.98
7.08		154.74	154.93	152.07	182.77	386.81	416.38	398.42	374.46	365.42	360.42	356.60	351.74
7.17		154.74	154.93	152.07	182.77	386.81	416.99	398.42	374.93	365.18	360.42	356.60	351.98
7.25		154.98	154.93	152.07	182.77	386.81	417.56	398.42	374.46	365.18	360.42	356.60	351.98
7.33		154.58	154.93	152.07	182.77	386.81	417.56	398.42	374.46	365.18	360.42	356.60	351.98
7.42		154.98	155.17	152.31	182.77	386.81	418.04	398.42	374.46	365.18	360.42	356.60	351.74
7.50		154.74	154.70	152.31	182.77	386.81	418.51	398.42	374.46	365.18	360.42	356.60	351.74
7.58		154.74	154.70	152.31	182.77	386.81	418.98	398.42	374.46	365.18	360.42	356.60	351.74
7.67		154.74	154.93	152.31	182.77	386.81	419.22	398.42	374.46	365.18	360.42	356.60	351.74
7.75		154.74	154.93	152.31	182.77	386.81	419.69	398.42	374.46	365.18	360.42	356.60	351.74
7.83		154.98	154.46	152.07	182.77	386.81	420.16	398.42	374.46	365.18	360.42	356.60	351.74
7.92		154.74	154.70	152.07	182.77	386.81	420.40	398.42	374.46	365.18	360.42	356.60	351.74
8.00		154.98	154.70	152.07	182.77	386.81	420.87	398.42	374.46	365.18	360.42	356.60	351.74
8.08		154.98	154.93	152.07	182.77	386.81	421.34	398.42	374.46	365.18	360.42	356.60	351.74
8.17		154.98	155.17	152.31	182.77	386.81	421.81	398.42	374.46	365.18	360.42	356.60	351.74
8.25		154.98	154.70	152.31	182.77	386.81	422.05	398.42	374.46	365.18	360.42	356.60	351.74
8.33		154.98	154.70	152.31	182.77	386.81	422.29	398.42	374.46	365.18	360.42	356.60	351.74
8.42		154.74	154.70	152.31	182.77	386.81	422.76	398.42	374.46	365.18	360.42	356.60	351.74
8.50		154.98	154.93	152.31	182.77	386.81	422.99	398.42	374.46	365.18	360.42	356.60	351.74
9.00		154.22	154.70	152.31	182.77	386.81	424.64	398.42	374.46	365.18	360.42	356.60	351.74
10.00		154.26	154.93	152.31	182.77	386.81	426.53	398.42	374.46	365.18	360.42	356.60	351.50
11.00		154.50	155.17	152.31	182.77	386.81	427.24	398.42	374.46	365.18	360.42	356.60	351.26
12.00		154.46	154.46	152.31	182.77	386.81	427.95	398.42	374.46	365.18	360.42	356.60	351.26
13.00		154.22	154.46	152.31	182.77	386.81	427.95	398.42	374.46	365.18	360.42	356.60	351.26
14.00		154.74	155.45	152.31	182.77	386.81	427.95	398.42	374.46	365.18	360.42	356.60	351.26
15.00		154.98	155.17	152.31	182.77	386.81	428.18	398.42	374.46	365.18	360.42	356.60	351.26
16.00		154.74	154.93	152.31	182.77	386.81	428.65	398.42	374.46	365.18	360.42	356.60	351.26
17.00		154.22	154.46	152.31	182.77	386.81	429.13	398.42	374.46	365.18	360.42	356.60	351.26
18.00		154.50	155.17	152.31	182.77	386.81	429.65	398.42	374.46	365.18	360.42	356.60	351.26
19.00		154.74	154.93	152.31	182.77	386.81	429.65	398.42	374.46	365.18	360.42	356.60	351.26
20.00		154.98	154.93	152.31	182.77	386.81	429.65	398.42	374.46	365.18	360.42	356.60	351.26
30.00		154.70	154.93	152.31	182.77	390.12	428.65	396.52	370.42	361.61	358.03	355.50	351.50

RUN 32A										
TIME (MIN)										
0	BATH1	BATH2	INLET	PELLET	2	3	4	5	6	7
1.00	355.17	354.22	351.83	378.50	381.59	410.24	402.20	376.84	366.61	361.13
2.00	355.41	353.74	351.59	378.50	381.35	410.71	402.20	376.84	366.37	361.13
3.00	355.17	354.22	351.59	378.26	381.35	411.19	401.97	376.60	366.37	361.13
4.00	354.43	354.22	351.83	378.26	381.35	411.42	402.44	376.36	366.13	360.89
5.00	355.17	355.17	351.59	378.26	381.35	411.19	402.68	376.60	366.37	361.13
5.25	355.65	354.70	351.59	378.26	381.35	411.42	402.68	376.60	366.37	361.13
5.33	355.89	355.17	351.59	378.26	381.35	410.95	402.68	376.36	366.37	360.89
5.42	355.65	354.93	351.59	378.26	381.59	411.66	402.91	376.36	366.37	360.89
5.50	355.41	354.70	351.59	378.50	381.82	412.13	403.15	376.36	366.37	361.13
5.58	355.15	354.46	351.83	378.50	381.42	412.61	403.39	376.60	366.37	361.13
5.67	355.41	353.98	351.83	378.74	382.06	413.08	403.86	376.84	366.61	361.13
5.75	355.65	353.74	351.83	378.74	382.06	413.31	404.10	376.84	366.61	361.13
5.83	354.70	353.98	351.83	378.74	382.30	414.02	404.33	377.07	366.61	361.13
5.92	354.93	353.98	351.83	378.74	382.30	414.49	404.33	377.07	366.61	361.13
6.00	354.93	354.22	351.59	378.97	382.30	414.73	404.57	377.31	366.61	361.13
6.08	354.93	353.78	351.83	378.97	382.30	414.97	404.80	377.07	366.85	361.13
6.17	354.93	354.22	351.83	378.97	382.53	415.44	405.04	377.07	366.61	361.13
6.25	354.93	354.46	351.93	378.97	382.53	416.15	405.28	377.31	366.61	361.13
6.33	354.93	354.46	351.83	378.97	382.53	416.62	405.28	377.31	366.61	361.13
6.42	355.17	353.74	351.83	379.21	382.53	416.86	405.51	377.31	366.61	361.13
6.50	354.70	354.22	351.83	379.21	382.53	417.33	405.51	377.31	366.61	361.13
6.58	354.70	354.22	351.83	379.21	382.77	417.56	405.75	377.55	366.61	361.13
6.67	355.17	354.22	351.83	379.21	382.77	418.04	405.75	377.31	366.61	361.13
6.75	355.41	354.22	351.83	379.21	382.77	418.27	405.75	377.55	366.61	361.13
6.83	354.93	354.22	351.83	379.21	382.77	418.98	405.99	377.31	366.61	361.13
6.92	354.93	354.22	351.83	379.21	382.77	419.22	405.99	377.07	366.37	360.89
7.00	354.93	353.98	351.83	379.45	383.01	419.89	405.99	377.31	366.37	360.89
7.08	354.70	354.46	351.83	379.45	383.01	419.93	405.99	377.07	366.37	360.89
7.17	354.93	354.70	351.83	379.45	383.01	420.16	405.99	376.84	366.37	360.89
7.25	355.17	355.17	351.83	379.45	383.01	420.63	405.99	376.84	366.13	360.89
7.33	355.17	354.70	351.83	379.45	383.01	420.67	405.99	376.84	366.13	360.89
7.42	355.17	354.70	351.83	379.45	383.01	421.34	405.99	376.84	366.13	360.66
7.50	354.93	354.70	351.83	379.45	383.01	421.58	405.99	376.84	366.13	360.66
7.58	355.17	354.46	351.83	379.45	383.01	422.05	405.99	376.60	366.13	360.66
7.67	354.93	354.22	351.83	379.45	383.01	422.29	405.99	376.60	366.13	360.66
7.75	354.93	354.46	351.83	379.45	383.01	422.52	405.99	376.60	366.13	360.66
7.83	355.17	354.22	351.83	379.45	383.01	422.99	405.99	376.60	366.13	360.66
7.92	355.17	354.22	351.83	379.45	383.01	423.23	405.99	376.36	366.66	360.42
8.00	355.41	354.46	351.83	379.45	383.01	423.70	405.99	376.12	366.66	360.42
8.08	355.17	354.22	351.83	379.45	383.01	423.94	405.99	376.12	366.66	360.42
8.17	354.93	354.22	351.83	379.45	383.01	424.17	405.99	376.12	366.66	360.42
8.25	354.70	353.98	351.83	379.45	383.01	424.41	405.99	376.12	366.42	360.42
8.33	354.93	354.22	351.83	379.45	383.01	424.64	405.99	375.89	366.42	360.18
8.42	354.93	354.70	351.83	379.21	383.01	425.35	405.99	375.41	366.18	360.18
9.00	354.70	353.98	351.83	379.21	382.77	427.00	405.75	374.70	364.47	359.70
10.00	354.93	354.70	351.83	379.21	382.77	430.07	405.51	373.51	363.99	359.46
11.00	354.70	354.22	351.83	379.21	382.77	431.95	405.04	373.03	363.28	359.99
12.00	355.65	354.46	351.83	379.45	383.01	433.60	404.80	372.80	363.04	358.75
13.00	354.93	353.98	352.07	379.69	383.48	434.31	404.80	372.32	362.80	358.27
14.00	354.70	353.98	352.07	379.92	383.48	434.78	404.10	372.32	362.56	358.27
15.00	354.93	353.98	351.83	379.92	383.48	435.02	403.62	371.61	362.32	358.27
16.00	354.46	354.46	351.83	379.69	383.48	435.72	403.39	371.61	362.32	358.27
17.00	354.93	354.70	351.83	379.45	383.25	436.43	403.15	371.37	362.32	358.27
18.00	355.41	354.22	351.83	379.45	383.25	437.14	402.91	371.61	362.32	358.27
19.00	355.65	354.46	352.07	379.21	383.01	437.61	403.15	371.61	362.56	358.27
20.00	355.89	354.22	351.83	379.45	383.25	437.61	403.39	371.61	362.09	358.27
30.00	354.70	353.98	351.83	380.16	383.96	436.67	402.91	370.89	361.85	358.03

RUN 328										
TIME (MIN)										
0	1	2	3	4	5	6	7	8	9	
1.00	353.96	381.35	439.73	399.60	360.70	360.09	357.56	349.93	352.79	
2.00	354.96	382.06	438.79	399.36	369.70	360.09	357.56	349.17	352.79	
3.00	355.98	382.06	438.32	398.89	369.70	361.37	357.56	349.17	352.79	
4.00	356.93	381.02	438.08	398.65	370.16	361.37	357.56	349.17	352.79	
5.00	356.17	381.95	438.79	398.65	369.23	361.37	357.56	349.41	352.79	
6.00	354.93	381.11	439.49	398.65	369.47	361.37	357.56	349.41	352.79	
7.00	354.93	381.11	439.73	398.42	369.47	361.37	357.56	349.41	352.79	
8.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
9.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
10.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
11.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
12.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
13.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
14.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
15.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
16.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
17.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
18.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
19.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
20.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	
30.00	354.93	381.11	439.73	398.65	369.47	361.37	357.56	349.41	352.79	

Appendix VIII TEMPERATURE PROFILE OF THE REACTOR WALL



Appendix IX CALCULATION OF THE ORDER OF REACTION

For a reaction system with a constant selectivity, the phthalic anhydride concentration can be expressed as

$$C_{pa} = k(C_o - C_x)$$

where C_o is the inlet o-xylene concentration

k is the selectivity

The rate of reaction containing inhibiting effects

$$R_r = \frac{k_r C_x}{1 + k_a C_{pa}}$$

can therefore be expressed as

$$R_r = \frac{k_r C_x}{1 + k_a k (C_o - C_x)}$$

which can be differentiated to determine the order of reaction

$$\frac{d(\ln R_r)}{d(\ln C_x)} = \frac{1 + k_a k C_o}{1 + k_a k (C_o - C_x)}$$

as $0 \leq k \leq 1$ and $C_o \geq C_x \geq 0$ the order of reaction must always be greater than or equal to 1, and can never be negative.

Similarly for the reaction model

$$R_r = k_r \frac{C_x^\alpha}{C_{pa}^\beta}$$

the order of reaction is given by

$$\frac{d(\ln R_r)}{d(\ln C_x)} = \frac{\beta + \alpha (C_o - C_x)}{C_o - C_x}$$

which is always positive for β and $\alpha > 0$

Appendix X

NORMALIZED PLOT OF REACTION MODELS

