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A special system of reaction equations

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ABSTRACT. A system of reaction equations describing polymer degradation is shown to be integrable in analytic terms.

1. Introduction

We consider a mathematical model for the degradation of polymers in an aqueous environment. The model describes the kinetics of polymer degradation by a set of ordinary differential equations which take into account the hydrolytic cleavage of a polymer autocatalyzed by acidic species produced during the degradation process. Processes of this type are of interest for the controlled release of drugs from polymer matrices (see [TH], [HG] for the biochemical background). Typical examples of biodegradable polymers are polylactids. The initial value problem for the ordinary differential equations modelling the degradation can of course be solved by standard numerical methods. A somewhat closer look – and the use of the computer algebra system "Maple" – showed that there are models where an explicit solution in analytical terms can be given.

The model is a very hypothetical one (see the remarks at the end of the text), it played an intermediate rôle in the development of a more realistic setting. Such a more realistic model has to take into account e.g. transport of material by diffusion.

2. The model equations

We make the usual assumption of elementary chemical kinetics that the concentrations of substances S_1, \dots, S_n develop in time t according to the differential equations

$$\frac{dS_k}{dt} = R_k(S_1, \dots, S_n), \quad k = 1, \dots, n \quad (2.1)$$

where the right hand sides R_k ($k = 1, \dots, n$) represent the rates of generation of the substances S_k . These terms express the stoichiometric relations between the reacting substances, they include reaction velocity constants.

We consider a model system with $n = 8$ where the substances (or species)

S_1, S_2, S_3, S_4, S_5 denote acid groups of different oligomers,

S_6 denotes the acid groups of the polymer,

S_7 denotes lactid,

S_8 denotes the ester groups of the polymer.

The corresponding reaction rates in (2.1) have the following structure:

$$\begin{aligned} R_1 &= 2c_0H(S_2 + S_3 + S_4 + S_5 + S_6), \\ R_2 &= c_0H(-S_2 + 2S_3 + 2S_4 + 2S_5 + 2S_6 + S_7), \\ R_3 &= c_0H(-2S_3 + 2S_4 + 2S_5 + 2S_6), \\ R_4 &= c_0H(-3S_4 + 2S_5 + 2S_6), \\ R_5 &= c_0H(-4S_5 + 2S_6), \\ R_6 &= c_0H(-10S_6 + S_8), \\ R_7 &= -2c_0HS_7, \\ R_8 &= -c_0H(20S_6 + S_8). \end{aligned}$$

Here c_0 denotes a reaction constant and H is defined by

$$H = c_1 W^{3/2} S^{1/2}, \text{ where } S = S_1 + S_2 + S_3 + S_4 + S_5 + S_6. \quad (2.2)$$

The acidity constant c_1 is given, W is the (saturation) water concentration within the polymer matrix. This structure of the reaction terms is motivated e.g. in [K], Chap.5. The reaction order is $3/2 + 1/2 + 1 = 3$.

In realistic situations the initial values at $t = 0$ are given as

$$\begin{aligned} S_1(0) &= S_2(0) = S_3(0) = S_4(0) = S_5(0) = 0, \\ S_6(0) &= S_6^{(0)}, S_7(0) = S_7^{(0)}, S_8(0) = S_8^{(0)}, \end{aligned}$$

with positive $S_6^{(0)}, S_7^{(0)}, S_8^{(0)}$. We introduce the so-called degree of polymerization P , a dimensionless quantity defined by

$$P = \frac{S_8}{S_6} + 1. \quad (2.3)$$

The name degree of polymerization is justified by the fact that this quantity decreases with time during the degradation process.

We eliminate S_8 using (2.3) and obtain

$$\left. \begin{aligned} \frac{dS_k}{dt} &= R_k(S_1, \dots, S_7, P), \quad k = 1, \dots, 7 \\ \frac{dP}{dt} &= -c_0 H(P^2 - 11P + 30). \end{aligned} \right\} \quad (2.4)$$

with the initial conditions

$$S_1(0) = S_2(0) = S_3(0) = S_4(0) = S_5(0) = 0, \quad S_6(0) = S_6^{(0)}, \quad S_7(0) = S_7^{(0)}, \quad P(0) = P_0$$

and with correspondingly transformed right hand sides

$$\begin{aligned} R_1 &= 2c_0 H(-S_2 + S_3 + S_4 + S_5 + S_6 + S_7), \\ R_2 &= c_0 H(-S_2 + 2S_3 + 2S_4 + 2S_5 + 2S_6 + S_7), \\ R_3 &= c_0 H(-2S_3 + 2S_4 + 2S_5 + 2S_6), \\ R_4 &= c_0 H(-3S_4 + 2S_5 + 2S_6), \\ R_5 &= c_0 H(-4S_5 + 2S_6), \\ R_6 &= c_0 H((P - 11)S_6), \\ R_7 &= -2c_0 H(S_7). \end{aligned}$$

which we wrote in a form showing the "diagonal" structure of the system. We can guarantee local (in time) existence of a chemically relevant solution.

Theorem 2.1. *For positive $S_6^{(0)}, S_7^{(0)}, S_8^{(0)}$ and $P_0 > 11$ there is a $T > 0$ such that the initial value problem (2.4) has a unique nonnegative solution on the time interval $[0, T]$.*

Proof. The right hand sides of (2.4) are continuous in R_1 and (locally) Lipschitz-continuous in $R_2, R_3, R_4, R_5, R_6, R_7, P$ on the nonnegative cone

$$C^+ = \{R_k \geq 0; k = 1, \dots, 7; P \geq 0\}.$$

Near the initial values the right hand sides are (locally) Lipschitz-continuous and existence and uniqueness of a solution follows from the classical theory (see e.g. [A]). A simple inspection of the equations reveals that the corresponding trajectories remain in C^+ on an appropriate time interval $[0, T), T > 0$. \square

3. Solution by analytical terms

The last equation of system (2.4) shows that we can introduce the degree of polymerization P as new independent variable. With $t = t(P)$ we obtain

$$\frac{dS_7}{dP} = \left(\frac{dS_7}{dt} \right) / \left(\frac{dP}{dt} \right) = \frac{2S_7}{P^2 - 11P + 30} = \frac{2S_7}{(P-5)(P-6)}.$$

The solution is (variables are "separable")

$$S_7(P) = S_7^{(0)} \left(\frac{P_0 - 5}{P_0 - 6} \right)^2 \left(\frac{P - 6}{P - 5} \right)^2.$$

In the same way we obtain from the equation for S_6 in (2.4) the equation

$$\frac{dS_6}{dP} = \left(\frac{dS_6}{dt} \right) / \left(\frac{dP}{dt} \right) = -\frac{S_6(P-11)}{P^2 - 11P + 30}$$

with the solution

$$S_6(P) = S_6^{(0)} \frac{(P_0 - 5)^6}{(P_0 - 6)^5} \frac{(P - 6)^5}{(P - 5)^6}.$$

With the substitutions $x = P - 5$, $b = P_0 - 5$ and

$$S_k(P) = S_k(x + 5) = Y_k(x), \quad k = 1, \dots, 7, \quad a = S_6^{(0)} \frac{b^6}{(b-1)^5}, \quad c = S_7^{(0)} \left(\frac{b}{b-1} \right)^2$$

we write these solutions in the form

$$Y_7(x) = c \left(\frac{x-1}{x} \right)^2, \quad Y_6(x) = a \frac{(x-1)^5}{x^6}.$$

Manipulating the equation for $k = 5$ in the same manner and using the substitutions just made we get for Y_5 the initial value problem

$$\frac{dY_5}{dx} = \frac{4Y_5 - 2Y_6}{x(x-1)}, \quad Y_5(b) = 0,$$

or, with the expression for Y_6 ,

$$\frac{dY_5}{dx} = \frac{4Y_5}{x(x-1)} - 2a \frac{(x-1)^4}{x^7}, \quad Y_5(b) = 0.$$

This linear inhomogeneous equation has the solution

$$Y_5(x) = \frac{a(b^2 - x^2)(x-1)^4}{b^2 x^6}.$$

Already here the calculations were controlled using the computer algebra system "Maple". Now the following steps are obvious: Climbing up the system from equation $k+1$ to equation k – which is possible thanks to the upper-diagonal structure of the system – we obtain linear inhomogeneous equations for Y_4, Y_3, Y_2 of increasing complexity and, finally, Y_1 by a quadrature.

For Y_4 we get the initial value problem

$$\frac{dY_4}{dx} = \frac{3Y_4 - 2Y_5 - 2Y_6}{x(x-1)}, \quad Y_4(b) = 0,$$

or, with the expression for Y_5, Y_6 ,

$$\frac{dY_4}{dx} = \frac{3Y_4}{x(x-1)} - 2a \frac{(x-1)^3}{x^6} \left(1 - \frac{x}{b^2}\right), \quad Y_4(b) = 0.$$

The solution is

$$Y_4(x) = \frac{a(x-1)^3(b-x)(b^2 + (b-2)x)}{b^3 x^5}.$$

For Y_3 we get

$$\frac{dY_3}{dx} = \frac{2(Y_3 - (Y_4 + Y_5 + Y_6))}{x(x-1)}, \quad Y_3(b) = 0,$$

and with

$$Y_4 + Y_5 + Y_6 = \frac{a(b-1)(x-1)^3(b^2 + b - 2x)}{b^3 x^4}$$

the linear inhomogeneous equation

$$\frac{dY_3}{dx} = \frac{2Y_3}{x(x-1)} - \frac{2a(b-1)(x-1)^2(b^2 + b - 2x)}{b^3 x^5}, \quad Y_3(b) = 0,$$

with the solution

$$Y_3(x) = \frac{a(b-1)(x-1)^2(b-x)(b^2 + b + (b-3)x)}{b^4 x^4}.$$

For Y_2 we get

$$\frac{dY_2}{dx} = \frac{Y_2 - 2(Y_3 + Y_4 + Y_5 + Y_6) - Y_7}{x(x-1)}, \quad Y_2(b) = 0,$$

and with

$$2(Y_3 + Y_4 + Y_5 + Y_6) + Y_7 = \frac{2a(b-1)^2}{b^4} \frac{(x-1)^2}{x^3} [b(b+2) - 3x] + c \frac{(x-1)^2}{x^2}$$

the linear inhomogeneous equation

$$\frac{dY_2}{dx} = \frac{Y_2}{x(x-1)} - \frac{(x-1)}{x^3} \left\{ \frac{2a(b-1)^2}{b^4} \frac{[b(b+2) - 3x]}{x} + c \right\}, \quad Y_2(b) = 0,$$

with the solution

$$Y_2(x) = \frac{(b-x)(x-1)}{b^5 x^3} \{ [cb^4 + a(b-1)^2(b-4)]x + ab(b-1)^2(b+2) \}.$$

For Y_1 we get

$$\frac{dY_1}{dx} = - \frac{2(Y_2 + Y_3 + Y_4 + Y_5 + Y_6)}{x(x-1)}, \quad Y_1(b) = 0,$$

and we could find Y_1 by a quadrature. The calculation can be simplified using

$$\frac{2(Y_2 + Y_3 + Y_4 + Y_5 + Y_6)}{x(x-1)} = 2 \frac{dY_2}{dx} + 3 \frac{dY_3}{dx} + 4 \frac{dY_4}{dx} + 5 \frac{dY_5}{dx} + \frac{30Y_6 + 2Y_7}{x(x-1)},$$

$$\frac{dY_7}{dx} = \frac{2Y_7}{x(x-1)},$$

which gives

$$\frac{dY_1}{dx} = - \left(2 \frac{dY_2}{dx} + 3 \frac{dY_3}{dx} + 4 \frac{dY_4}{dx} + 5 \frac{dY_5}{dx} + \frac{dY_7}{dx} + \frac{30Y_6}{x(x-1)} \right).$$

Integration yields with the initial conditions

$$Y_1(b) = Y_2(b) = Y_3(b) = Y_4(b) = Y_5(b) = 0, \quad Y_6(b) = S_6^{(0)}, \quad Y_7(b) = S_7^{(0)}:$$

$$Y_1(x) = Y_7(b) - Y_7(x) - 2Y_2(x) - 3Y_3(x) - 4Y_4(x) - 5Y_5(x) + 30 \int_x^b \frac{Y_6(\xi)}{\xi(\xi-1)} d\xi.$$

We put

$$J(x) = 30 \int_x^b \frac{Y_6(\xi)}{\xi(\xi-1)} d\xi = 30a \int_x^b \frac{(\xi-1)^4}{\xi^7} d\xi$$

and obtain with

$$J(x) = 30a(j(1/b) - j(1/x)), \quad \text{where } j(y) = y^2 \left(-\frac{1}{2} + \frac{4}{3}y - \frac{3}{2}y^2 + \frac{4}{5}y^3 - \frac{1}{6}y^4 \right),$$

for Y_1 the representation

$$Y_1(x) = Y_7(b) - Y_7(x) - 2Y_2(x) - 3Y_3(x) - 4Y_4(x) - 5Y_5(x) + J(x).$$

To complete our programme we have still to solve the second equation (2.4) to establish a relation between the time t and the (translated) degree of polymerization x . We put in (2.2) $K = c_0 c_1 W^{3/2}$ and obtain in the new variables x, Y_k :

$$t = \frac{1}{K} \int_x^b \frac{d\xi}{\xi(\xi-1)\sqrt{Y(\xi)}}, \quad \text{where } Y = Y_1 + Y_2 + Y_3 + Y_4 + Y_5 + Y_6.$$

We substitute $\eta = 1/\xi$ and get with $z = 1/x$

$$t = \frac{1}{K} \int_{1/b}^z \frac{d\eta}{(1-\eta)\sqrt{Y(1/\eta)}}. \quad (3.1)$$

An inspection shows that Y_1, \dots, Y_7 are polynomials in $y = 1/x$ of degree at most 6, i.e. they have the form

$$Y_k(y) = A_k + B_k y + C_k y^2 + D_k y^3 + E_k y^4 + F_k y^5 + G_k y^6, \quad (k = 1, \dots, 7).$$

So we can expect that in (3.1) appears a hyperelliptic integral. A closer ("Maple"-supported) analysis reveals that also this integral reduces to an elementary one. A comparison of coefficients shows for Y_6, Y_5, Y_4, Y_3

$$\begin{aligned} A_6 &= 0, & A_5 &= -\frac{a}{b^2}, & A_4 &= \frac{a(2-b)}{b^3}, & A_3 &= \frac{a(b-1)(3-b)}{b^4}, \\ B_6 &= a, & B_5 &= \frac{4a}{b^2}, & B_4 &= \frac{a(b-6)}{b^3}, & B_3 &= -\frac{2a(b-1)(b+3)}{b^4}, \\ C_6 &= -5a, & C_5 &= \frac{a(b^2-6)}{b^2}, & C_4 &= \frac{a(b^3+3b+6)}{b^3}, & C_3 &= \frac{a(b-1)(b^3+b^2+7b+3)}{b^4}, \\ D_6 &= 10a, & D_5 &= \frac{4a(1-b^2)}{b^2}, & D_4 &= -\frac{a(b^3+5b+2)}{b^3}, & D_3 &= -\frac{2a(b-1)(b^2+b+2)}{b^3}, \\ E_6 &= -10a, & E_5 &= \frac{a(b^2-6)}{b^2}, & E_4 &= \frac{a(3b^2+2)}{b^3}, & E_3 &= \frac{a(b^2-1)}{b^2}, \\ F_6 &= 5a, & F_5 &= -4a, & F_4 &= -a, & F_3 &= 0, \\ G_6 &= -a, & G_5 &= -a, & G_4 &= 0, & G_3 &= 0. \end{aligned}$$

For Y_2 we find $E_2 = F_2 = G_2 = 0$ and

$$\begin{aligned} A_2 &= -\frac{1}{b^5} (cb^4 + a(b-1)^2(b-4)), & B_2 &= \frac{c(b+1)}{b} - \frac{a(b-1)^2(5b+4)}{b^5}, \\ C_2 &= -c + \frac{a(b-1)^2(b^2+2b+6)}{b^4}, & D_2 &= -\frac{a(b-1)^2(b+2)}{b^3}, \end{aligned}$$

for Y_1

$$\begin{aligned} A_1 &= Y_7(b) - c + 30aj(1/b) - 2A_2 - 3A_3 - 4A_4 - 5A_5, \\ B_1 &= 2c - 2B_2 - 3B_3 - 4B_4 - 5B_5, \\ C_1 &= c - 15a - 2C_2 - 3C_3 - 4C_4 - 5C_5, \end{aligned}$$

$$\begin{aligned}
D_1 &= -40a - 2D_2 - 3D_3 - 4D_4 - 5D_5, \\
E_1 &= 45a - 3E_3 - 4E_4 - 5E_5 = 0, \\
F_1 &= -24a - 4F_4 - 5F_5 = 0, \\
G_1 &= 5a - 5G_5 = 0.
\end{aligned}$$

The corresponding polynomial for $Y = Y_1 + Y_2 + Y_3 + Y_4 + Y_5 + Y_6$ is

$$Y(y) = A + By + Cy^2 + Dy^3 + Ey^4 + Fy^5 + Gy^6$$

with

$$\begin{aligned}
A &= \sum_{k=1}^6 A_k, & B &= \sum_{k=1}^6 B_k, & C &= \sum_{k=1}^6 C_k, & D &= \sum_{k=1}^6 D_k, \\
E &= \sum_{k=1}^6 E_k, & F &= \sum_{k=1}^6 F_k, & G &= \sum_{k=1}^6 G_k.
\end{aligned}$$

Computation of these sums gives

$$C = D = E = F = G = 0$$

and

$$A = -\left(\frac{Y_7(b)}{b-1} + \frac{5a(b-1)^4}{b^6}\right), \quad B = \frac{Y_7(b)b}{b-1} + \frac{a}{b^5}(b-1)^4(b+4).$$

Remembering that $a = S_6^{(0)} \frac{b^6}{(b-1)^5}$, $Y_7(b) = S_7^{(0)}$ we can write

$$A = -\frac{5S_6^{(0)} + S_7^{(0)}}{b-1}, \quad B = \frac{b}{b-1} ((b+4)S_6^{(0)} + S_7^{(0)}), \quad (3.2)$$

which shows that $A < 0$, $B > 0$ and $|B/A| > 1$ because of $b > 1$. So the integral in (3.1) gets the announced elementary form and we have

$$t = t(z) = \frac{1}{K} \int_{1/b}^z \frac{d\eta}{(1-\eta)\sqrt{A+B\eta}} = \frac{1}{K\sqrt{|A|}} \int_{1/b}^z \frac{d\eta}{(1-\eta)\sqrt{\beta\eta-1}}, \quad \beta = \frac{B}{|A|} > 1.$$

With

$$\int \frac{d\eta}{(1-\eta)\sqrt{\beta\eta-1}} = \frac{2}{\sqrt{\beta-1}} \operatorname{arctanh} \sqrt{\frac{\beta\eta-1}{\beta-1}}, \quad \text{where } \operatorname{arctanh} w = \frac{1}{2} \log \left(\frac{1+w}{1-w} \right),$$

we get

$$t = t(z) = \frac{2}{K\sqrt{B+A}} \left\{ \operatorname{arctanh} \sqrt{\frac{Bz+A}{B+A}} - \operatorname{arctanh} \sqrt{\frac{B/b+A}{B+A}} \right\}. \quad (3.3)$$

By (3.2) and $P_0 = b + 5$ we have $A + B = S_7^{(0)} + P_0 S_6^{(0)}$ and $B/b + A = S_6^{(0)}$. We put

$$w = \sqrt{\frac{Bz + A}{B + A}}, \quad w_0 = \sqrt{\frac{B/b + A}{B + A}}$$

and inverting (3.3) we find

$$w(t) = \frac{1 - \left(\frac{1-w_0}{1+w_0}\right) \exp(-K\sqrt{A+B}t)}{1 + \left(\frac{1-w_0}{1+w_0}\right) \exp(-K\sqrt{A+B}t)} \quad (3.4)$$

and hence

$$z = z(t) = \frac{1}{B} \left\{ (B + A)w^2(t) - A \right\}. \quad (3.5)$$

Remembering $x = 1/z$ and $P = x+5$ we have the explicit time-dependence of the degree of polymerization $P = P(t)$ and, finally, of the concentrations $S_k = S_k(t)$, ($k = 1, \dots, 7$). We summarize:

Theorem 3.1. *For $P_0 \geq 6$ the solution of system (2.4) exists $\forall t \geq 0$. With the function $z = z(t)$ defined by (3.4), (3.5) the degree of polymerization is $P(t) = 5 + (1/z(t))$, the (nonnegative) concentrations $S_k = S_k(t)$, ($k = 1, \dots, 7$) are polynomials in z of degree at most 6.*

4. Asymptotics

Written in the variable z we have

$$\begin{aligned} S_7(z) &= c(1-z)^2, \quad S_6(z) = az(1-z)^5, \quad S_5(z) = \frac{a}{b^2}(b^2z^2-1)(1-z)^4 \\ S_4(z) &= \frac{a}{b^3}(bz-1)(b^2z+b-2)(1-z)^3, \quad S_3(z) = \frac{a}{b^4}(bz-1)(b(b+1)z+b-3)(1-z)^2, \\ S_2(z) &= \frac{1}{b^5}(bz-1) \left\{ ab(b-1)^2(b+2)z + cb^4 + a(b-1)^2(b-4) \right\} (1-z), \\ S_1(z) &= S_7(b) - S_7(z) + 30a(j(1/b) - j(z)) - 2S_2(z) - 3S_3(z) - 4S_4(z) - 5S_5(z). \end{aligned}$$

where

$$j(z) = z^2 \left(-\frac{1}{2} + \frac{4}{3}z - \frac{3}{2}z^2 + \frac{4}{5}z^3 - \frac{1}{6}z^4 \right).$$

These formulae allow precise statements on the asymptotic behaviour as $t \rightarrow \infty$. From (3.4), (3.5) follows

$$0 \leq 1 - w(t) \leq 2 \left(\frac{1-w_0}{1+w_0} \right) \exp(-K\sqrt{A+B}t), \quad 1 - z = \frac{A+B}{B}(1-w^2),$$

consequently we have exponential decay

$$w(t) \rightarrow 1, \quad z(t) \rightarrow 1 \text{ as } t \rightarrow \infty.$$

With the foregoing formulae follows

Theorem 4.1. *For $t \rightarrow \infty$ the solution of (2.4) tends to the asymptotic state*

$$\begin{aligned} P(\infty) &= 6, \quad S_1(\infty) = S_7^{(0)} + 30a \left(j \left(\frac{1}{b} \right) + \frac{1}{30} \right), \\ S_2(\infty) &= S_3(\infty) = S_4(\infty) = S_5(\infty) = S_6(\infty) = S_7(\infty) = 0. \end{aligned}$$

Remark 4.1. The asymptotic behaviour is just the expected one: At the "end" of the degradation process only the "smallest" oligomer with the "smallest" degree of polymerization is present. The powers of $1 - z$ in the expressions of the oligomer concentrations S_2, S_3, S_4, S_5, S_6 show that the concentrations of oligomers with higher index decay faster. (See the corresponding curves.)

Remark 4.2. The possibility to construct a solution by elementary expressions depends on the diagonal structure of the right hand sides R_1, \dots, R_7 and on the simple fact that the reaction constant c_0 is the same in all equations. If e.g. in the equation for S_7 the constant c_0 is substituted by $c_2 \neq c_0$ (the interesting case is $c_2 \gg c_0$), we get for the (correspondingly transformed) quantity Y_7 the expression

$$Y_7(x) = c^* \left(\frac{x-1}{x} \right)^{2c_2/c_0} \quad \text{with} \quad c^* = S_7^{(0)} \left(\frac{b}{b-1} \right)^{2c_2/c_0}.$$

In this case it is in general impossible to find Y_2, Y_1, t by elementary expressions. Nevertheless, we have in this case essentially the same asymptotics as expressed in Theorem 4.1, with the only difference that

$$S_1(\infty) = \frac{c_0}{c_2} S_7^{(0)} + 30a \left(j \left(\frac{1}{b} \right) + \frac{1}{30} \right).$$

Remark 4.3. We add some curves using the initial values

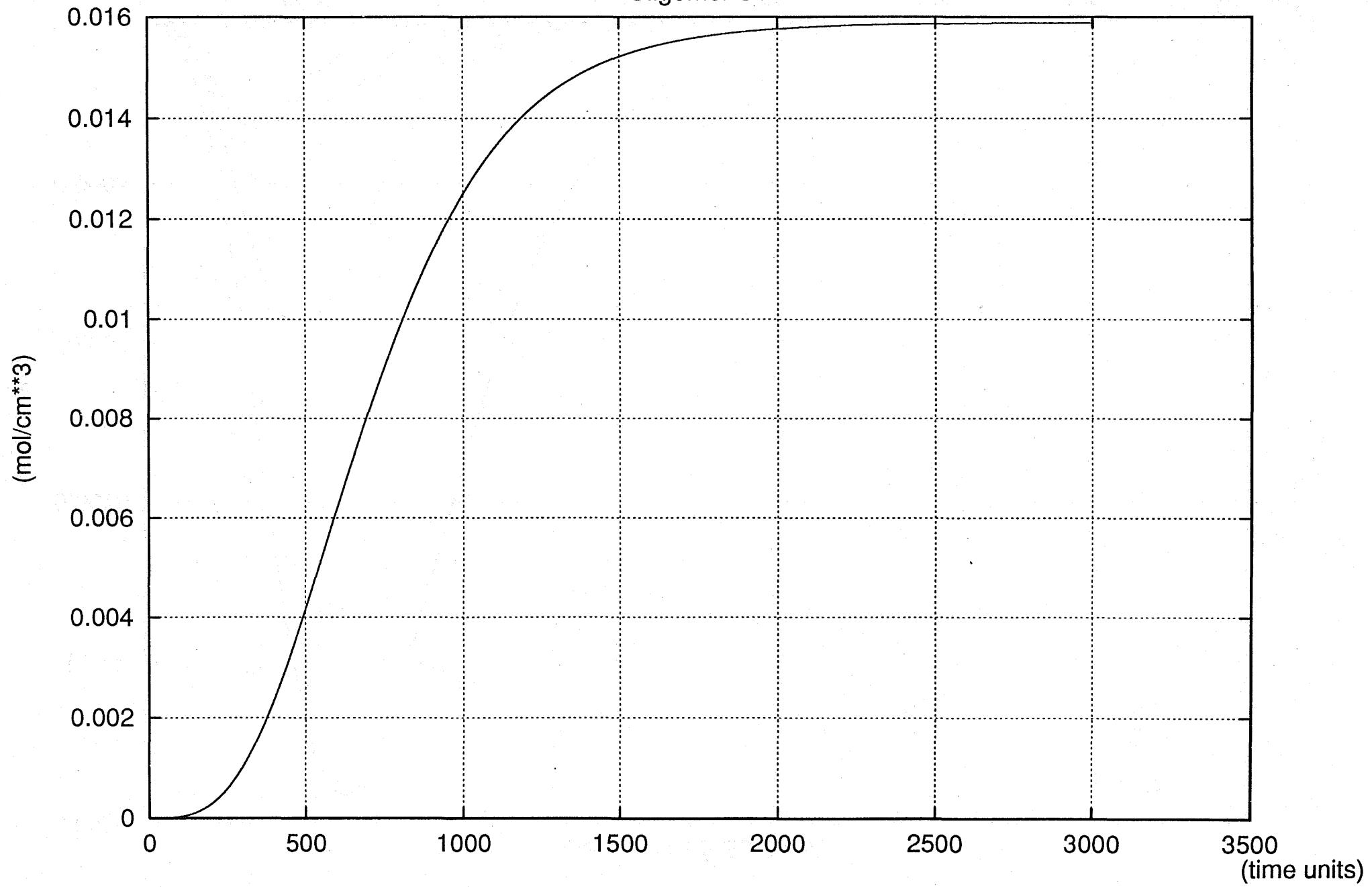
$$S_6^{(0)} = 0.28975 \cdot 10^{-4}, \quad S_7^{(0)} = 0.7892 \cdot 10^{-3}, \quad S_8^{(0)} = 0.15067 \cdot 10^{-1},$$

where the natural unit for concentrations is $\text{mol} \cdot \text{cm}^{-3}$. Therefore the initial value for the degree of polymerization is $P_0 = 521$. The time scale has to be interpreted corresponding to the choice of the reaction constant c_0 . The curves show the qualitative behaviour mentioned in Remark 4.1.

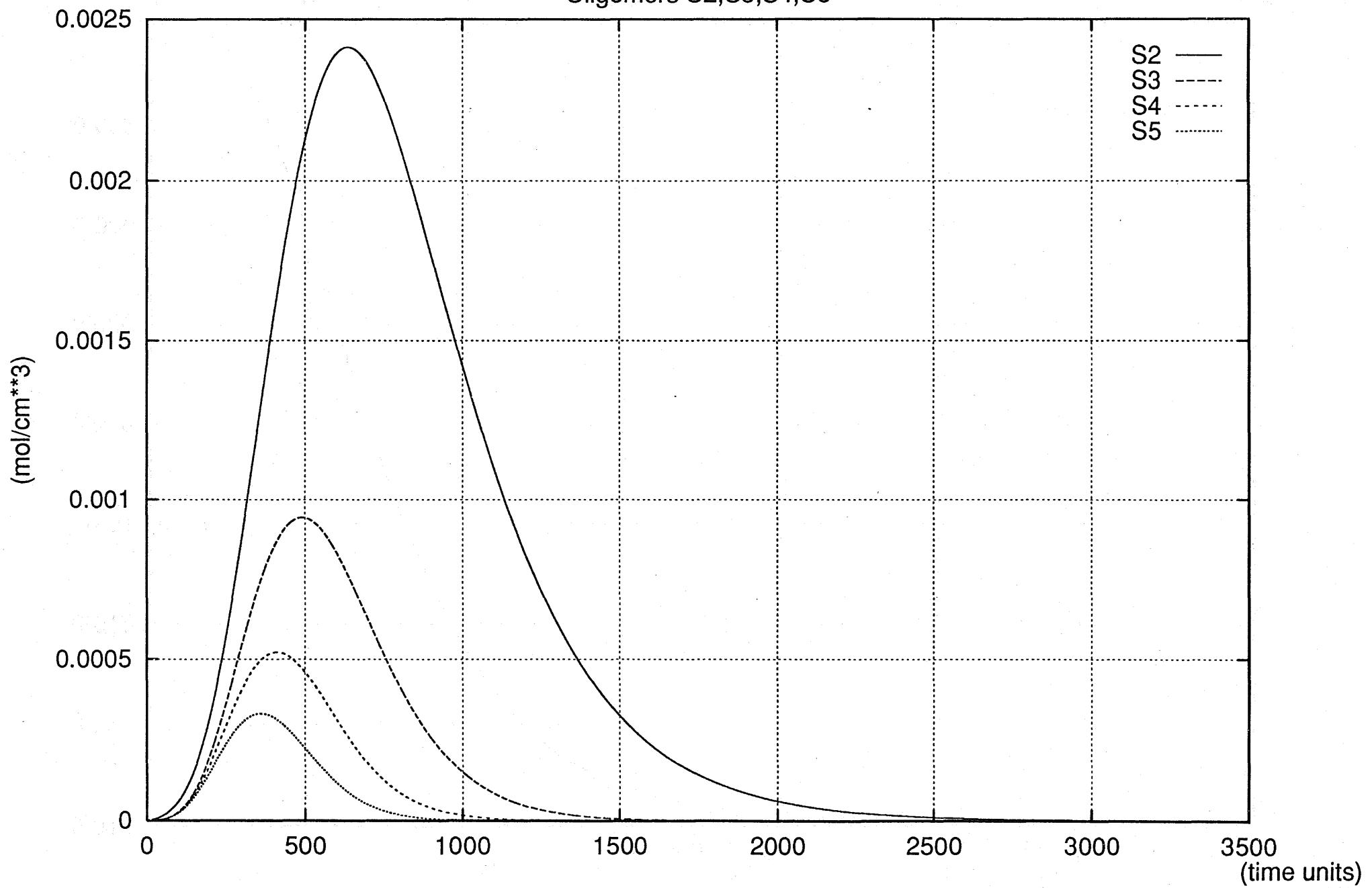
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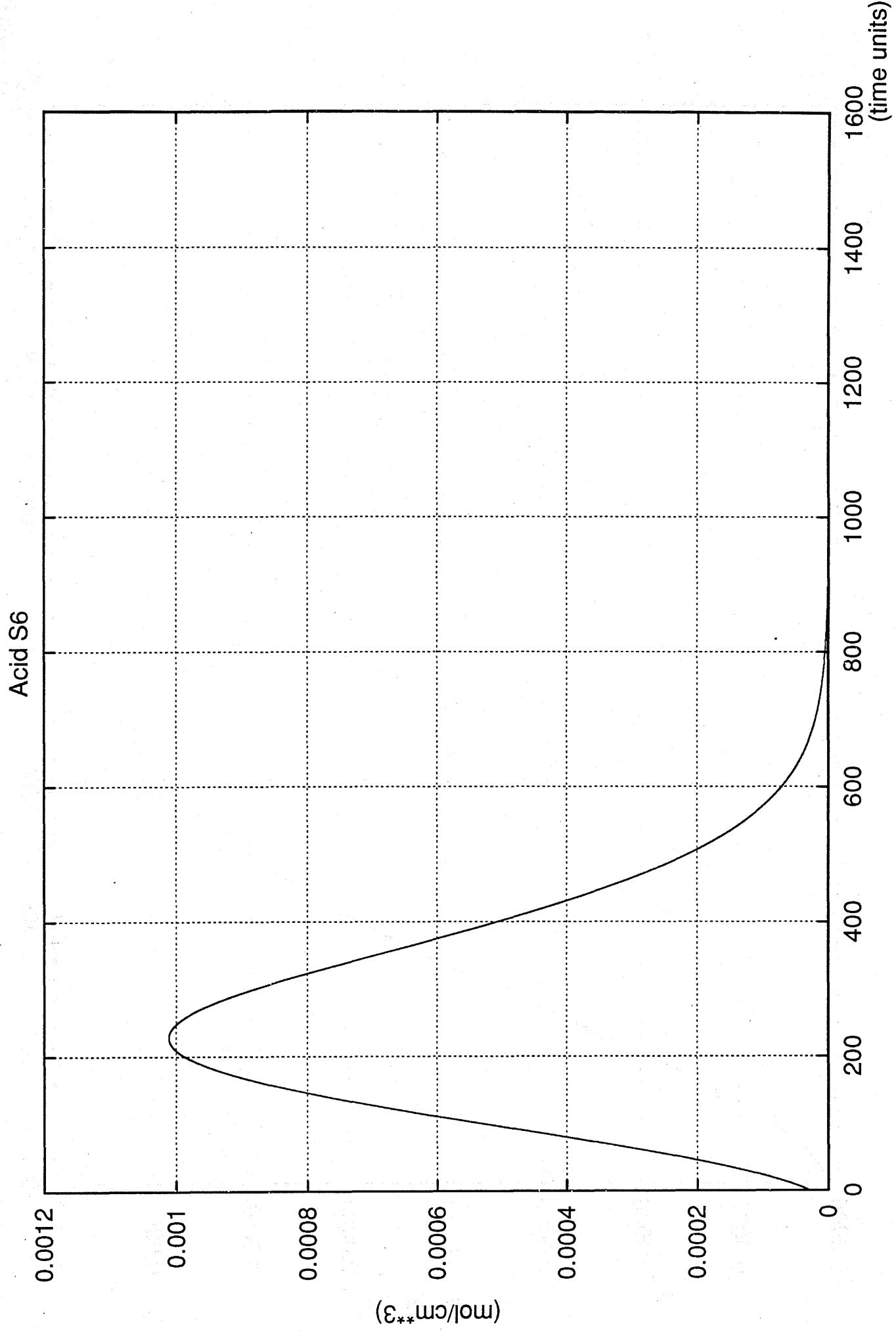
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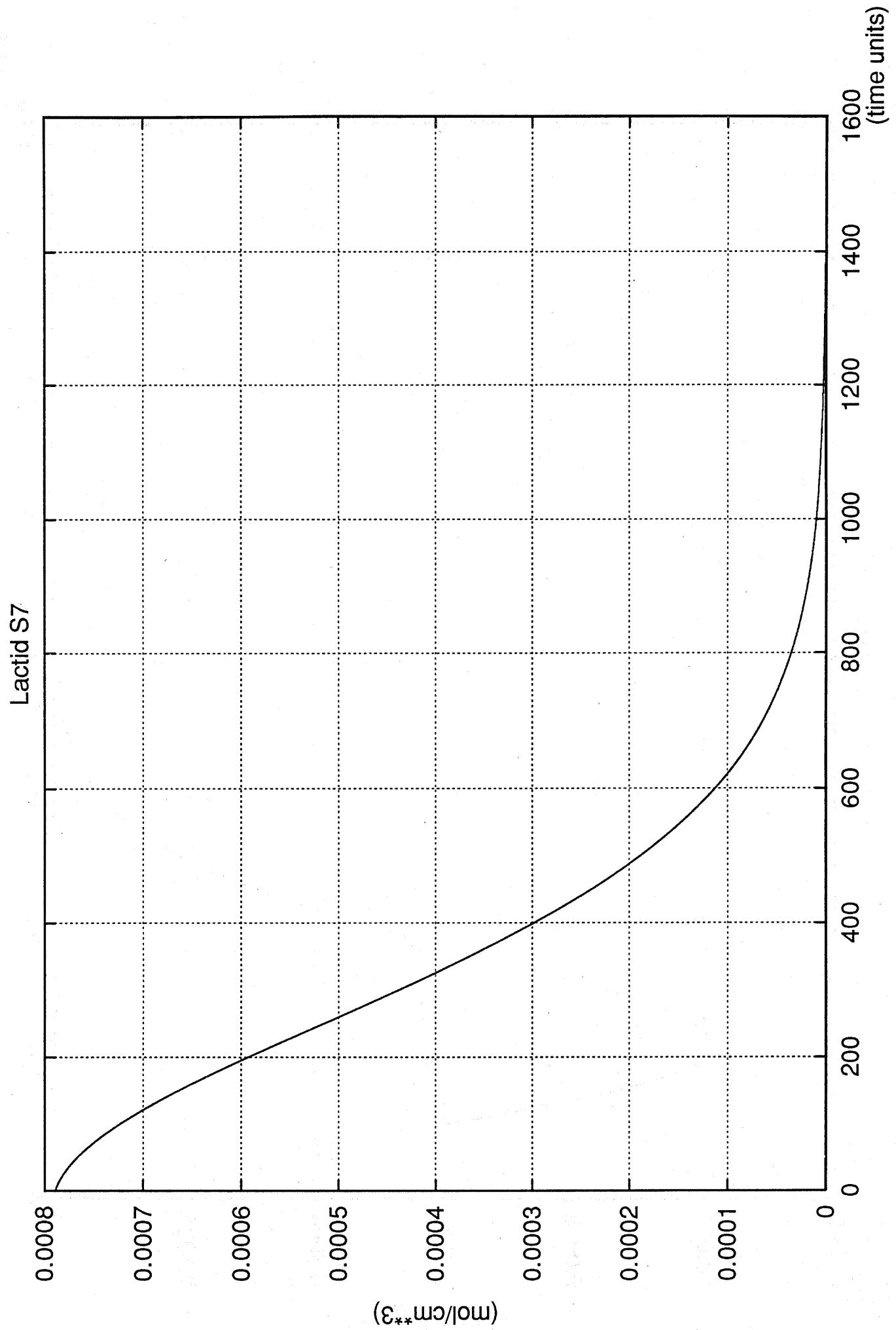
Oligomer S1

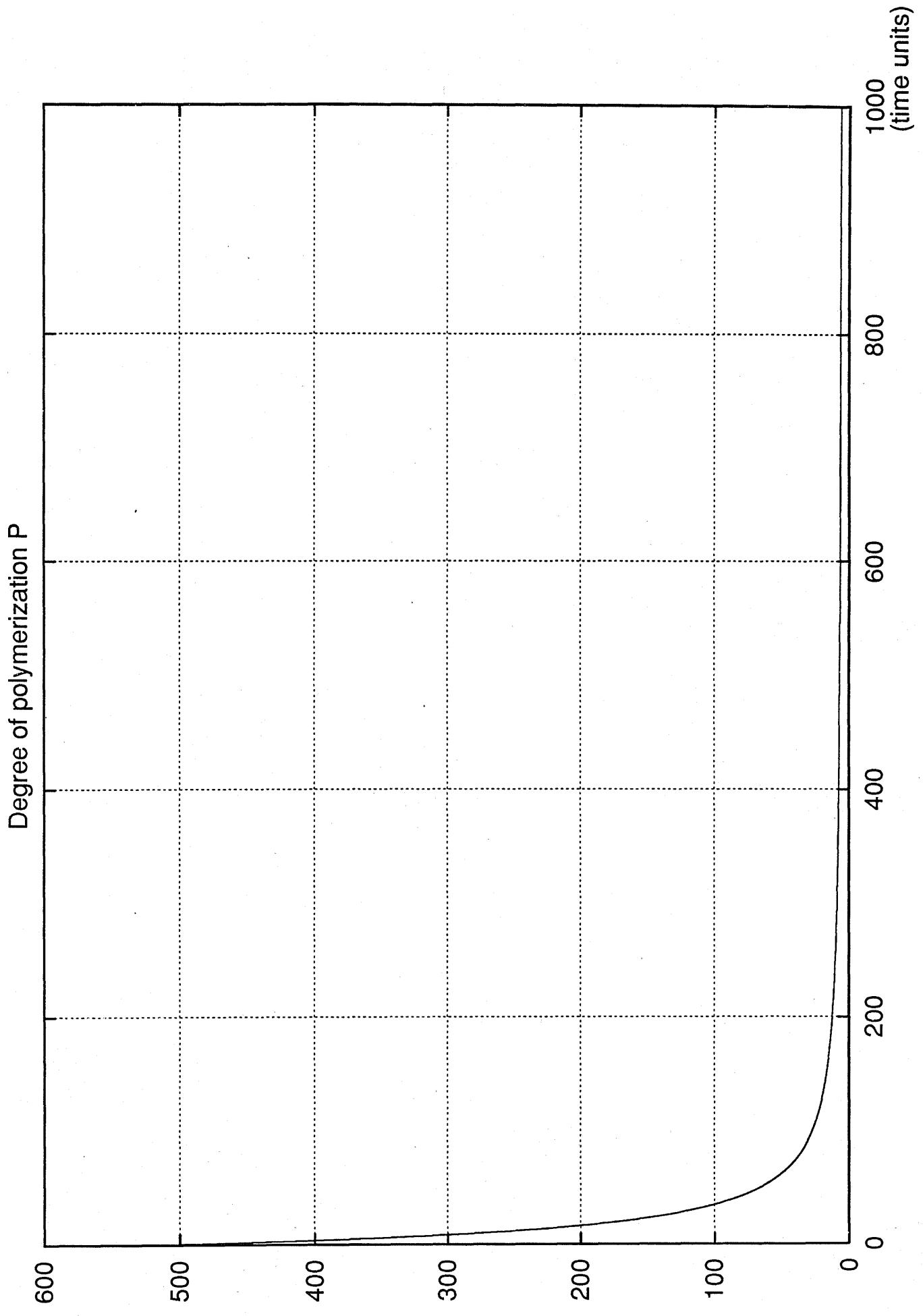


Oligomers S2,S3,S4,S5









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