

DEVELOPMENT OF A SECOND-ORDER CLOSURE MODEL
FOR COMPUTATION OF TURBULENT DIFFUSION FLAMES

Ashok K. Varma and Coleman duP. Donaldson

Prepared under Contract No. NAS1-12412

by

Aeronautical Research Associates of Princeton, Inc.
50 Washington Road, Princeton, New Jersey 08540

for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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ABSTRACT

A "typical eddy" box model for the second-order closure of turbulent, multi-species, reacting flows has been developed. The model structure is quite general and is valid for an arbitrary number of species. For the case of a reaction involving three species, the nine model parameters are determined from equations for the nine independent first- and second-order correlations: $\bar{\alpha}$, $\bar{\beta}$, \bar{T} , $\overline{\alpha'\beta'}$, $\overline{\alpha'\gamma'}$, $\overline{\beta'\gamma'}$, $\overline{\alpha'T'}$, $\overline{\beta'T'}$, and $\overline{T'T'}$. The model enables calculation of any higher-order correlation involving mass fractions, temperatures, and reaction rates in terms of first- and second-order correlations. Model predictions for the reaction rate are in very good agreement with exact solutions of the reaction rate equations for a number of assumed flow distributions.

INTRODUCTION

Recent advances in the analysis of turbulent flows by closure of the transport equations for various Reynolds stresses at the second-order level have resulted in a deeper understanding of the physics of turbulent flows that could not be obtained by classical first-order closure methods such as the eddy viscosity method. A.R.A.P. has been in the forefront of the application of second-order modeling techniques to the calculation of turbulent shear flows. We have successfully applied these techniques to a variety of flow problems including incompressible and compressible free shear layers and boundary layers (ref. 1), simulation of the flow in a HF chemical laser (ref. 2); behavior of the planetary boundary layer (ref. 3); and the decay of axisymmetric vortices (ref. 4). In the course of these studies, we have developed and tested models for a large number of third-order correlations that appear in the transport equations for the second-order correlations. These models will have direct application in our current development of a computer program to analyze turbulent reacting flows.

The analysis of turbulent, multi-species, reacting flows is an example of the kind of problem that requires a more sophisticated approach than the eddy viscosity method. During the past two years, A.R.A.P. has been developing an invariant second-order coupled

diffusion and chemistry model with support from NASA, EPA, and DOT. The model has been used to study a number of atmospheric (incompressible) chemistry problems such as the dispersal of pollutants from industrial stacks and highways, the behavior of the far wake of the SST exhaust, and other similar problems (ref. 5). These studies demonstrated that there are indeed real world atmospheric pollution problems in which neglect of the fluctuations of concentrations of reacting species introduces significant errors. Neglect of the effects of inhomogeneous mixing could result in order of magnitude errors in the chemical reaction rates. An approximate closure scheme for the chemical submodel which conforms to the principles of invariant modeling and which accounts for the effects of inhomogeneous mixing over a wide range of conditions was developed.

The above-mentioned studies of modeling of reacting flows were limited to problems involving low heat release in which the fluctuations in the reaction rate could be neglected. However, the success of these studies raised the distinct possibility that by combining the compressible flow models with further advances in chemical modeling, it will be possible to construct a second-order closure model for the computation of compressible flow problems involving highly exothermic chemical reactions, such as the analysis of a turbulent diffusion flame. A.R.A.P. is currently being funded by NASA under Contract NAS1-12412 to develop the models for third-order correlations involving fluctuations of species concentrations, temperatures, and reaction rates. This report details the development of these models over the past year.

CHEMICAL KINETIC EQUATIONS

Consider an irreversible single-step reaction between chemical species α and β to form γ .



We will primarily deal with such a three-species system, although the model can easily be extended to reactions involving more species; for example,



The reaction rate equations may be written

$$\frac{\partial[\alpha]}{\partial t} = -k[\alpha][\beta] \quad (2)$$

$$\frac{\partial[\beta]}{\partial t} = -k[\alpha][\beta]$$

If, instead of the molar concentrations $[\alpha]$ and $[\beta]$, Eqs. (2) are written in terms of the mass fractions α and β , the reaction equations become

$$\frac{\partial \alpha}{\partial t} = -k_1 \alpha \beta \quad k_1 = k \frac{\rho}{W_\beta} \quad (3)$$

$$\frac{\partial \beta}{\partial t} = -k_2 \alpha \beta \quad k_2 = k \frac{\rho}{W_\alpha} \quad (4)$$

where ρ is the density, W_α and W_β are the molecular weights of species α and β , respectively, and k_1 and k_2 are the reaction rate constants.

Equations (3) and (4) specify the local instantaneous rate of change of the concentration of the reactants. In a turbulent reacting flow, these equations may be written in terms of the mean and fluctuating values by writing a given quantity ϕ as the sum of a mean and fluctuating part

$$\phi = \bar{\phi} + \phi' \quad (5)$$

If Eqs. (3) and (4) are expanded by the scheme given in (5), the result is

$$\begin{aligned} \frac{\partial \bar{\alpha}}{\partial t} + \frac{\partial \alpha'}{\partial t} &= -(\bar{k}_1 + k_1')(\bar{\alpha} + \alpha')(\bar{\beta} + \beta') \\ &= -(\bar{k}_1 + k_1')(\bar{\alpha}\bar{\beta} + \bar{\alpha}\beta' + \bar{\beta}\alpha' + \alpha'\beta') \end{aligned} \quad (6)$$

and

$$\frac{\partial \bar{\beta}}{\partial t} + \frac{\partial \beta'}{\partial t} = -(\bar{k}_2 + k_2')(\bar{\alpha}\bar{\beta} + \bar{\alpha}\beta' + \bar{\beta}\alpha' + \alpha'\beta') \quad (7)$$

The chemical kinetic equations for the average rates of change of the concentrations of α and β then become

$$\frac{\partial \bar{\alpha}}{\partial t} = -\bar{k}_1(\bar{\alpha}\bar{\beta} + \overline{\alpha'\beta'}) - \bar{\alpha} \overline{k_1'\beta'} - \bar{\beta} \overline{k_1'\alpha'} - \overline{k_1'\alpha'\beta'} \quad (8)$$

and

$$\frac{\partial \bar{\beta}}{\partial t} = -\bar{k}_2(\bar{\alpha}\bar{\beta} + \overline{\alpha'\beta'}) - \bar{\alpha} \overline{k_2'\beta'} - \bar{\beta} \overline{k_2'\alpha'} - \overline{k_2'\alpha'\beta'} \quad (9)$$

In a second-order closure scheme, one generally carries equations for all the independent second-order correlations of the fluctuations. Chemical kinetic equations can be easily derived for terms such as $\overline{\alpha'\beta'}$ as follows. By subtracting Eqs. (8) and (9) from (6) and (7), respectively, one obtains

$$\begin{aligned} \frac{\partial \alpha'}{\partial t} = & - \bar{k}_1 \bar{\alpha} \beta' - \bar{k}_1 \bar{\beta} \alpha' - \bar{k}_1 (\alpha' \beta' - \overline{\alpha' \beta'}) - \bar{\alpha} \bar{\beta} k_1' \\ & - \bar{\alpha} (k_1' \beta' - \overline{k_1' \beta'}) - \bar{\beta} (k_1' \alpha' - \overline{k_1' \alpha'}) - (k_1' \alpha' \beta' - \overline{k_1' \alpha' \beta'}) \end{aligned} \quad (10)$$

$$\begin{aligned} \frac{\partial \beta'}{\partial t} = & - \bar{k}_2 \bar{\alpha} \beta' - \bar{k}_2 \bar{\beta} \alpha' - \bar{k}_2 (\alpha' \beta' - \overline{\alpha' \beta'}) - \bar{\alpha} \bar{\beta} k_2' \\ & - \bar{\alpha} (k_2' \beta' - \overline{k_2' \beta'}) - \bar{\beta} (k_2' \alpha' - \overline{k_2' \alpha'}) - (k_2' \alpha' \beta' - \overline{k_2' \alpha' \beta'}) \end{aligned} \quad (11)$$

Multiplying (10) by β' , (11) by α' , and averaging the sum of the resulting expressions

$$\begin{aligned} \frac{\partial}{\partial t} \overline{\alpha' \beta'} = & \overline{\beta' \frac{\partial \alpha'}{\partial t} + \alpha' \frac{\partial \beta'}{\partial t}} \\ = & - k_1 (\bar{\alpha} \overline{\beta' \beta'} + \bar{\beta} \overline{\alpha' \beta'} + \overline{\alpha' \beta' \beta'}) \\ & - \bar{\alpha} \bar{\beta} \overline{k_1' \beta'} - \bar{\alpha} \overline{k_1' \beta' \beta'} - \bar{\beta} \overline{k_1' \alpha' \beta'} - \overline{k_1' \alpha' \beta' \beta'} \\ & - \bar{k}_2 (\bar{\alpha} \overline{\alpha' \beta'} + \bar{\beta} \overline{\alpha' \alpha'} + \overline{\alpha' \alpha' \beta'}) \\ & - \bar{\alpha} \bar{\beta} \overline{k_2' \alpha'} - \bar{\alpha} \overline{k_2' \alpha' \beta'} - \bar{\beta} \overline{k_2' \alpha' \alpha'} - \overline{k_2' \alpha' \alpha' \beta'} \end{aligned} \quad (12)$$

Expressions for other independent second-order correlations can be obtained in a similar fashion. Equations (8), (9), and (12) contain higher-order correlations, such as the terms $\overline{\alpha' \beta' \beta'}$, $\overline{k_1' \alpha' \beta'}$, $\overline{k_2' \alpha' \beta'}$, $\overline{k_1' \alpha' \alpha'}$, $\overline{k_1' \alpha' \beta' \beta'}$, etc., which now have to be modeled in terms of the mean quantities $\bar{\alpha}$, $\bar{\beta}$, \bar{T} , etc., and the second-order correlations $\overline{\alpha' \beta'}$, $\overline{\alpha' \alpha'}$, $\overline{\beta' \gamma'}$, $\overline{\alpha' T'}$, etc. Once all the higher-order terms are modeled, we have a closed system of equations for the means and the independent second-order correlations which can be solved. We now have to develop suitable models for the various higher-order correlations.

"TYPICAL EDDY" BOX MODEL

In the second-order closure of the chemical submodel for a reacting mixture of three species, let us identify what information is available to us to construct a general model for the higher-order correlations and what the constraints are on the model.

Some effort was devoted to the development of analytical model expressions for the third-order correlations following procedures similar to those used in reference 5 for low heat release reactions. These were not entirely successful because of the lack of proper bounds on third-order terms like $\overline{k'\alpha'\alpha'}$. It was decided to construct a "typical eddy" for modeling concentration, temperature, and reaction rate fluctuations. A similar concept is used for modeling other correlations. For example, dissipation of turbulent kinetic energy is modeled as though all the dissipation was due to eddies of a single scale length. The tendency towards isotropy is modeled in terms of another scale length, and so on.

First, let us consider how many variables are at our disposal to construct the model of a "typical eddy" for the chemistry submodel. We have the equations for the mean terms

$$\bar{\alpha}, \bar{\beta}, \text{ and } \bar{T} \quad (13)$$

Note that $\bar{\gamma}$ is not an independent variable since

$$\bar{\alpha} + \bar{\beta} + \bar{\gamma} \equiv 1$$

Further, we have equations for

$$\overline{\alpha'\beta'}, \overline{\alpha'\gamma'}, \overline{\beta'\gamma'}, \overline{\alpha'T'}, \overline{\beta'T'}, \text{ and } \overline{T'^2} \quad (14)$$

These are the only species and/or temperature second-order correlations that are independent since $\alpha' + \beta' + \gamma' \equiv 0$ and, therefore,

$$\begin{aligned} \overline{\alpha'^2} &= - (\overline{\alpha'\beta'} + \overline{\alpha'\gamma'}) \\ \overline{\beta'^2} &= - (\overline{\alpha'\beta'} + \overline{\beta'\gamma'}) \\ \overline{\gamma'^2} &= - (\overline{\alpha'\gamma'} + \overline{\beta'\gamma'}) \\ \overline{\gamma'T'} &= - (\overline{\alpha'T'} + \overline{\beta'T'}) \end{aligned}$$

We note that if we have $\overline{\alpha'T'}$ or $\overline{\beta'T'}$, since the reaction rate terms k_1 and k_2 are known functions of T (for example, an Arrhenius relationship), we should be able to write expressions for $\overline{k_1'\alpha'}$, $\overline{k_1'\beta'}$, etc. One of our problems in selecting

a model is to obtain expressions for $\overline{k_1'\alpha'}$, $\overline{k_1'\alpha'\beta'}$, etc. in terms of the known quantities (13) and (14) which are completely consistent with our expressions for $\overline{\alpha'T'}$ and $\overline{\alpha'\beta'T'}$.

As listed above, we have nine independent parameters (Eqs. (13) and (14)) to construct a typical eddy for a mixture of three species. If we remain at a particular place in a fluid and watch the turbulent flow go by and ask, "What does a typical eddy look like?" or "What is the typical repetitive structure of the flow?", the answer will be some variation of the following. Consider two unmixed streams of α and β , which mix and react to form γ . In the early stages of the mixing, one will observe large amounts of pure α and β . Some reaction would have occurred and some pure product γ may pass by. There would be diffusion taking place and we expect to observe fluid elements consisting of differing proportions of $\alpha + \beta$ and $\alpha + \beta + \gamma$ (wherein the reaction is proceeding), $\alpha + \gamma$ and $\beta + \gamma$. At a later time, one would expect less frequent fluid masses consisting of pure α and β but the basic structure of the eddy will be the same. With this physical and intuitive idea of the flow, we now try to construct a model. The degrees of freedom of the model are limited by the number of independent parameters available.

Let us also set down other desirable features of the model and certain constraints the model must satisfy.

1. The three-species model should be capable of collapsing to the case of one or two species and be logically extendible to larger number of species.
2. The model should not have to label the three species; that is, which are the reactants and which are the products? Further, the model should be capable of handling a nonreacting mixture of three constituents.
3. The model must satisfy the end of the reaction constraints; that is, if $\bar{\alpha}$ and $\bar{\beta}$ are the reactants,

$$\overline{\alpha'\beta'} = -\bar{\alpha} \cdot \bar{\beta}$$

$$\overline{\alpha'^2\beta'} = \bar{\alpha}^2\bar{\beta} - \overline{\alpha'^2\beta}$$

Consider now the model for a mixture of three species. In the absence of any temperature fluctuations, there are only five independent parameters with which to construct the typical eddy. These are

$$\bar{\alpha}, \bar{\beta}, \overline{\alpha'\beta'}, \overline{\alpha'\gamma'}, \text{ and } \overline{\beta'\gamma'} \quad (15)$$

A desirable "typical eddy" structure, shown in Figure 1a, requires as many as 11 parameters, $\epsilon_1 \rightarrow \epsilon_6$ and $k_4 \rightarrow k_8$.

Obviously, we cannot have this general a model. A large number of simpler models were investigated. The proportions of the various materials in cells 4 through 7 can be fixed first. If cell 7, in which α , β , and γ exist together, is part of the model, cells 4, 5, and 6 could be considered to have either equal amounts of the two constituents or have them in proportion to the mean concentrations. In order to be able to consider the case of nonreacting mixing of three species for which the end result is a uniformly mixed flow, the concentrations in cell 7 must be proportional to the mean values. If cell 7 is taken out of the model (this cell is only absolutely necessary for accurate computation when the reaction rates are slow compared to diffusion processes), the concentrations in cells 4, 5, and 6 must be in proportion to the mean values, for the model should be capable of handling a confined flame in which the reactants are not available in stoichiometric proportions. Then, the end result is a uniformly mixed flow of $\bar{\alpha}$ and $\bar{\gamma}$ (or $\bar{\beta}$ and $\bar{\gamma}$) and the amounts of α and γ in cell 5 should be proportional to the means. By symmetry, we must do the same for cells 4 and 6.

With the above-noted assumptions, we have six unknowns, $\epsilon_1 \rightarrow \epsilon_6$, in the model. Various possible models were investigated. Some of the models which were rejected are sketched in Figures 1b and 1c. These failed for different reasons - lack of symmetry, not satisfying the reaction end limit, etc.

After extensive studies, we were left with two models which met all the conditions and tests we applied to them and appeared to be quite satisfactory. The predictions of these models were compared to the true chemistry results for a number of assumed flow distributions, and the results were very good. The models and the tests are discussed later in this report.

Both of these models were a significant improvement over "classical" chemistry calculations, but in some flows Model I showed better results while Model II did better in other flows. A seven cell, six parameter model combining the better features of these two models appeared to be desirable, but it would require an additional independent parameter, and we could not find a consistent way of introducing another parameter. In the last month we have developed a new seven-cell model (Model III) which still requires only five parameters. This model is discussed in a later section "Description of Model III." It must be tested more completely in the same way that Models I and II were tested, but the final model is so closely related to these two models that we expect it to show very similar results.

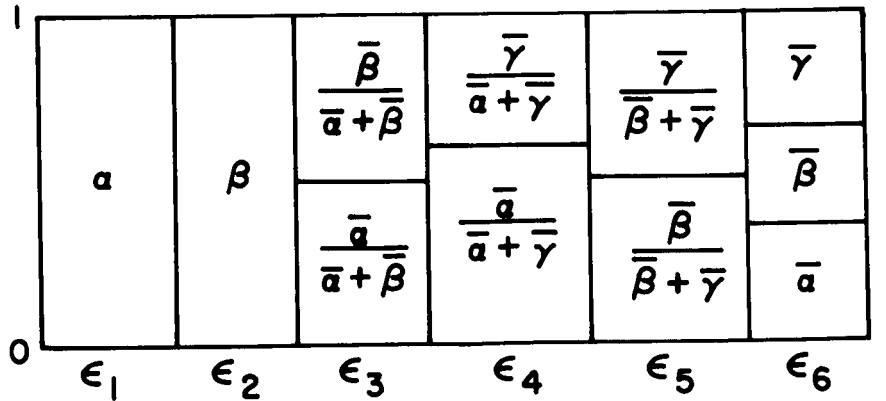
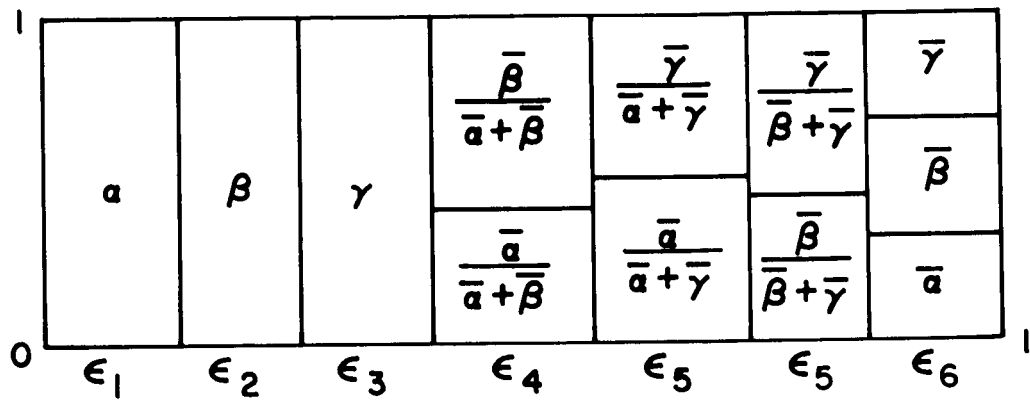
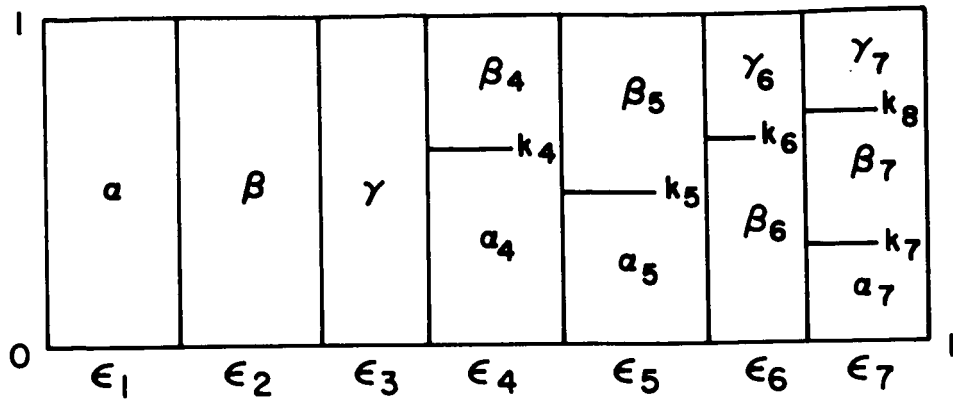


Figure 1. Some of the rejected "typical eddy" cell models

DISCUSSION OF MODELS I AND II

We now consider the joint species temperature models. With no temperature fluctuations, there are five parameters ($\bar{\alpha}$, $\bar{\beta}$, $\overline{\alpha'\beta'}$, $\overline{\alpha'\gamma'}$, $\overline{\beta'\gamma'}$) for the three-component species model. For variable temperatures, we have four additional parameters (\bar{T} , $\overline{T'T'}$, $\overline{\alpha'T'}$, $\overline{\beta'T'}$). For a mixture of two species, we have a total of five parameters: $\bar{\alpha}$, $\overline{\alpha'\beta'}$, \bar{T} , $\overline{T'T'}$, $\overline{\alpha'T'}$. For the case when only one species is present, the model must admit temperature fluctuations whose distribution functions are almost Gaussian, and to allow this result we assume that in the temperature distribution functions each cell spends one-half its time at a temperature ΔT above its base temperature. In the case of one species, the ΔT is governed by wall boundary conditions and/or viscous heating within the shear layer. The one- and two-species models are shown in Figure 2.

The six cell, three-species models I and II are shown in Figures 3 and 4. The temperature model has four unknowns: T_α , T_β , T_γ , and ΔT . The temperatures of the other three cells are the appropriately weighted means of the three base temperatures for the three species.

The concentration model and the temperature model allows one to compute any higher-order correlation of scalar fluctuations involving concentrations or temperatures. The second and higher-order correlations involving the fluctuations of the reaction rate constant k' can also be calculated, because it is possible to calculate the instantaneous reaction rate k and plot the reaction rate distributions for each half cell as shown in the figure. Then it is possible to calculate $k'\alpha'$, $k'\beta'$ or any other higher-order correlation of k' with fluctuations in concentration or temperature.

The three-species models described above have been compared against exact solutions of the reaction rate equations. The procedure is as follows. A number of base flows (assumed concentration and temperature distributions) are set up. A computer program has been written to calculate the nine model parameters from the values of the nine first- and second-order correlations for a given base flow at specified modeling times. The program then calculates various moments for the base flow as the reactions proceed in time. A comparison of the model predictions and the base flow (or true) chemistry is displayed using a plotting routine.

The following reaction rate expression has been used for the tests reported here:

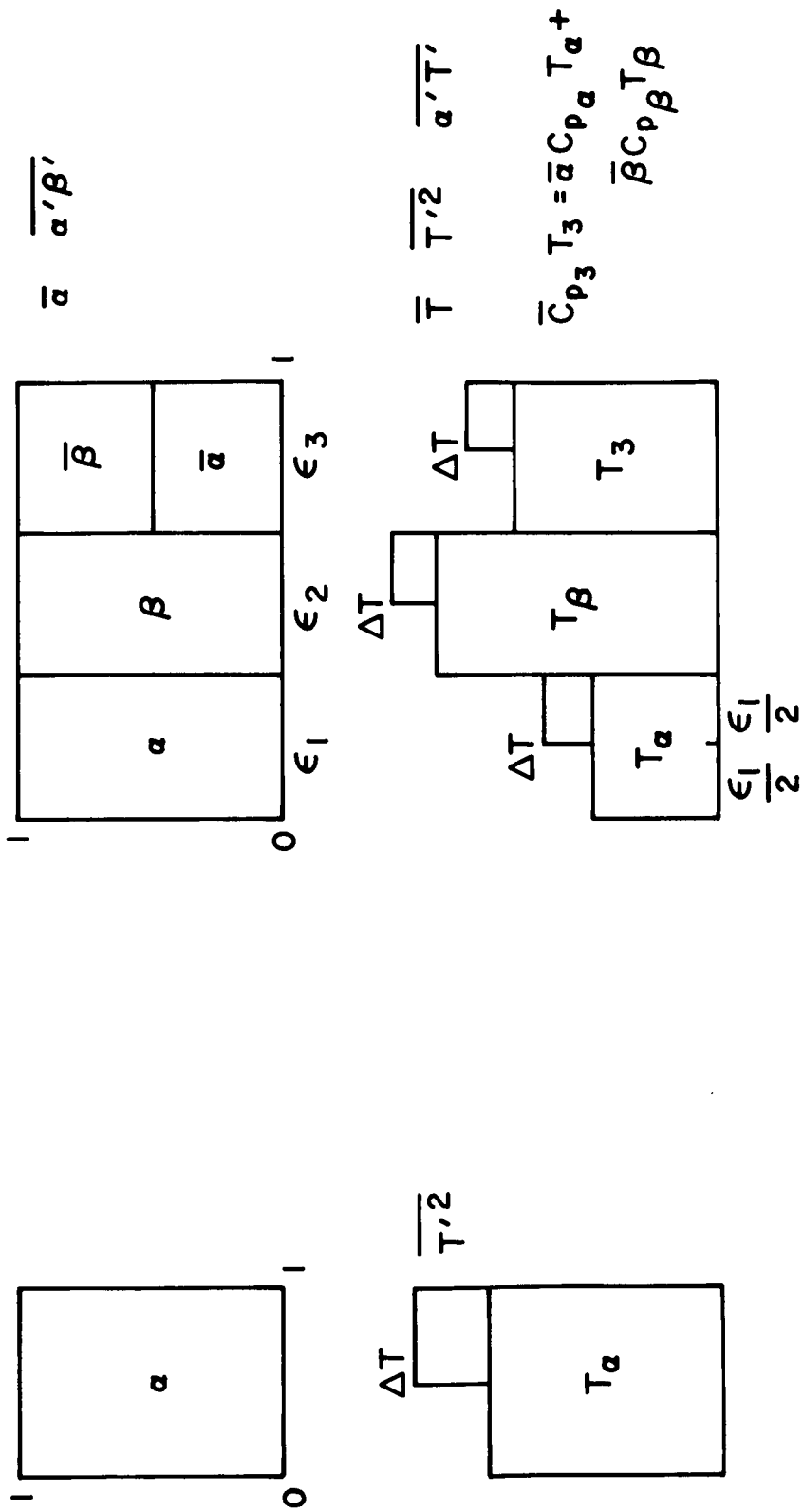
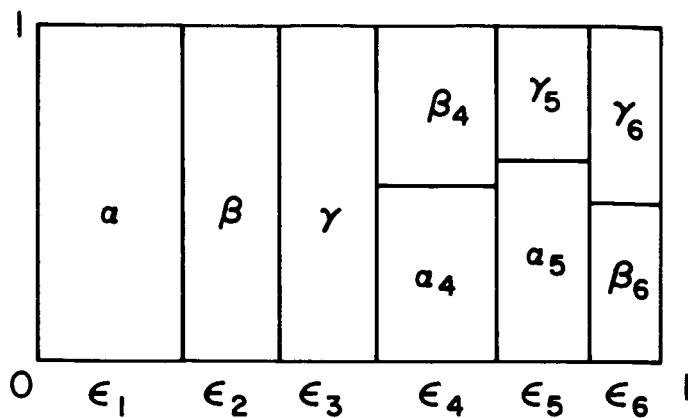


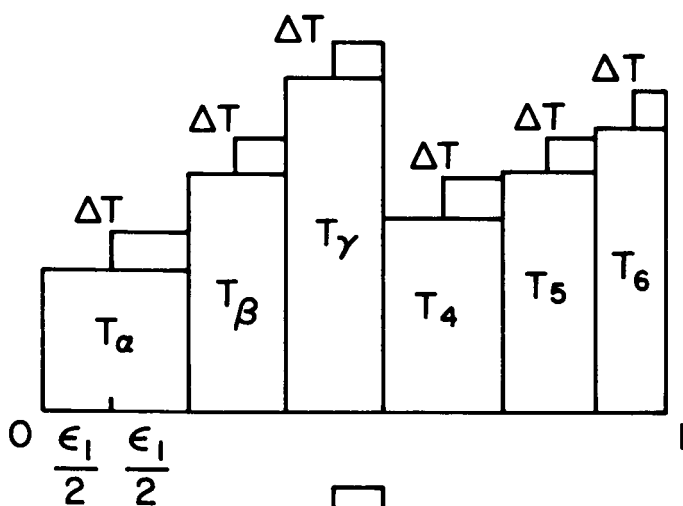
Figure 2. Typical eddy cell models for one and two species



$$\bar{\alpha}, \bar{\beta}, \overline{\alpha'\beta'}, \overline{\alpha'\gamma'}, \overline{\beta'\gamma'}$$

$$\alpha_4 = \bar{\alpha} / \bar{\alpha} + \bar{\beta} \quad \alpha_5 = \bar{\alpha} / \bar{\alpha} + \bar{\gamma}$$

$$\beta_4 = \bar{\beta} / \bar{\alpha} + \bar{\beta} \quad \beta_6 = \bar{\beta} / \bar{\beta} + \bar{\gamma}$$

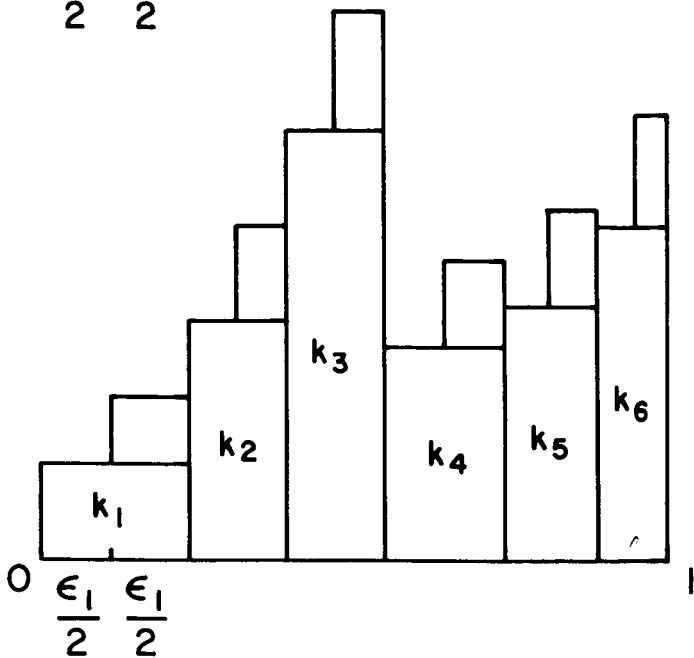


$$\bar{T}, \overline{T^2}, \overline{\alpha'T'}, \overline{\beta'T'}$$

$$\bar{C}_{p4} T_4 = \alpha_4 C_{p\alpha} T_\alpha + \beta_4 C_{p\beta} T_\beta$$

$$\bar{C}_{p5} T_5 = \alpha_5 C_{p\alpha} T_\alpha + \gamma_5 C_{p\gamma} T_\gamma$$

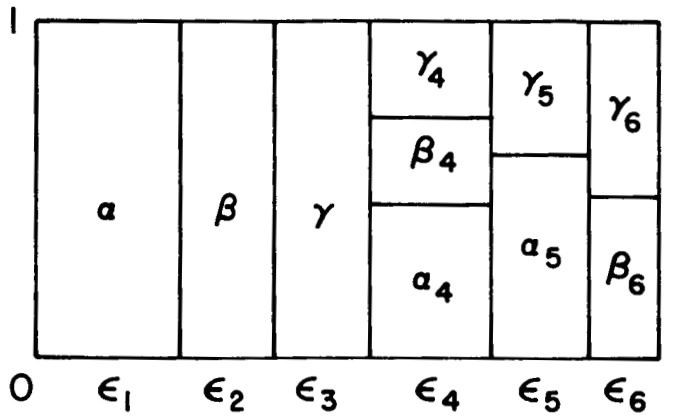
$$\bar{C}_{p6} T_6 = \beta_6 C_{p\beta} T_\beta + \gamma_6 C_{p\gamma} T_\gamma$$



$$k_i = A T_i^n \exp\left(-\frac{E_A}{R T_i}\right)$$

note $\bar{k} \neq k(\bar{T})$

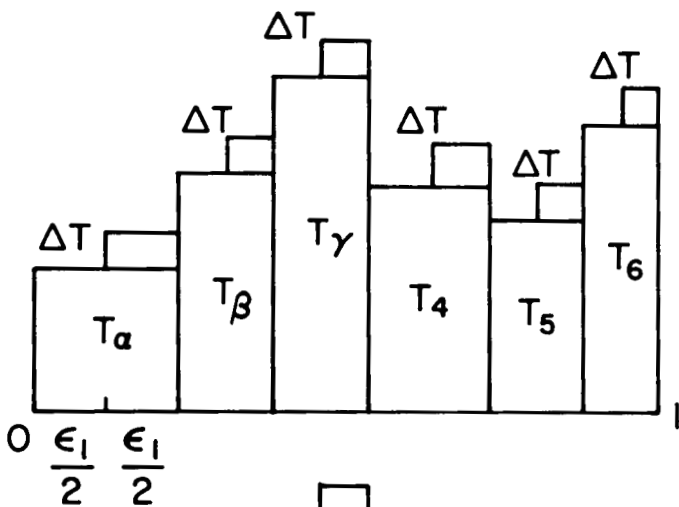
Figure 3. Model I for a typical eddy in three-species flow



$$\bar{a}, \bar{\beta}, \overline{a'\beta'}, \overline{a'\gamma'}, \overline{\beta'\gamma'}$$

$$a_4 = \bar{a} \quad a_5 = \bar{a} / \bar{a} + \bar{\gamma}$$

$$\beta_4 = \bar{\beta} \quad \beta_6 = \bar{\beta} / \bar{\beta} + \bar{\gamma}$$

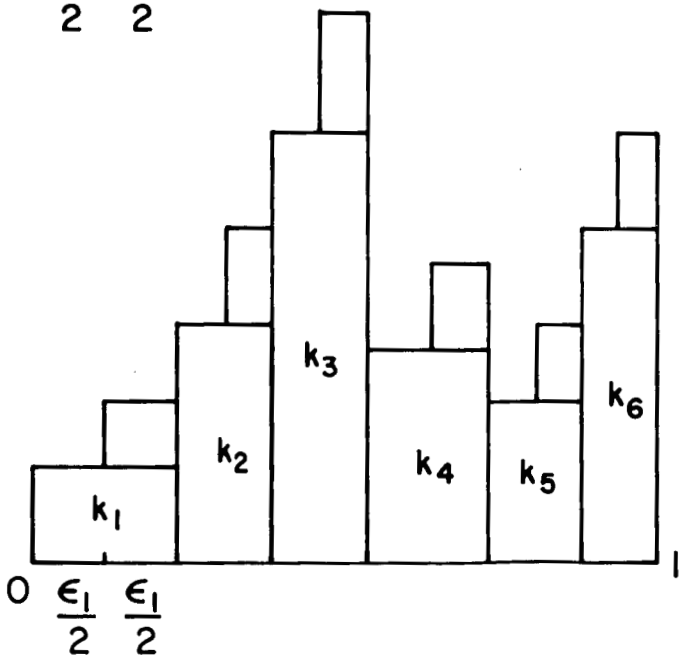


$$\bar{T}, \overline{T'^2}, \overline{a'T'}, \overline{\beta'T'}$$

$$\bar{C}_{p4} T_4 = a_4 C_{p\alpha} T_\alpha + \beta_4 C_{p\beta} T_\beta + \gamma_4 C_{p\gamma} T_\gamma$$

$$\bar{C}_{p5} T_5 = a_5 C_{p\alpha} T_\alpha + \gamma_5 C_{p\gamma} T_\gamma$$

$$\bar{C}_{p6} T_6 = \beta_6 C_{p\beta} T_\beta + \gamma_6 C_{p\gamma} T_\gamma$$



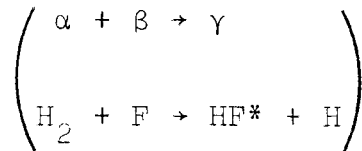
$$k_i = A T_i^n \exp\left(-\frac{E_A}{RT_i}\right)$$

$$\text{note } \bar{k} \neq k(\bar{T})$$

Figure 4. Model II for a typical eddy in three-species flow

$$k = 1.5 \times 10^{14} \exp\left(-\frac{1600}{RT}\right)$$

This corresponds to the reaction



in a HF chemical laser. A.R.A.P. is studying the turbulent mixing and reaction in these devices with support from ARPA.

Figure 5 shows first the influence of various terms in the expression for $\partial\bar{\alpha}/\partial t$ (eq. (8)). An exact solution of the chemical kinetic equations was obtained for base flow 1, and all the moments of interest were generated. The graph clearly illustrates the importance of taking the second-order $k'\alpha'$ and $k'\beta'$, and the third-order $k'\alpha'\beta'$ correlation into account for predicting the reaction rate.

Figures 6 and 7 present the results of modeling base flow 1 for the variable temperature and the constant temperature cases. The parameters of the base flow are shown on the figure. The "classical" chemistry results are obtained as $\partial\bar{\alpha}/\partial t = k(\bar{T}) \cdot \bar{\alpha} \cdot \bar{\beta}$; that is, by ignoring the turbulent fluctuations. Models I and II are established at time zero from the parameters of the base flow distribution function and the models are then allowed to proceed in time. It can be seen that the inclusion of temperature fluctuations leads to larger differences between the classical and true results. The model predictions in both cases show a very significant improvement over the classical results, but Model I is definitely superior for this flow.

Results for three other base flows are presented in Figures 8 through 13. For base flow 2, the selected temperatures are quite high, and the reaction rate values are virtually saturated. Consequently, Figures 8 (variable temperatures) and 9 (constant temperatures) do not exhibit large differences. The model flows are markedly better than classical chemistry calculations in both cases, but Model I does better in one case while Model II follows better the true chemistry result in the other case. For base flow 3, the results shown in Figures 10 and 11 indicate that Model I is superior to Model II. Finally, for base flow 4, we see that for the variable temperature case (fig. 12), Model II would be the preferred model, but the constant temperature studies in Figure 13 suggest that Model I is the better model.

In all these cases studied, the model predictions are significantly better than classical chemistry calculations and

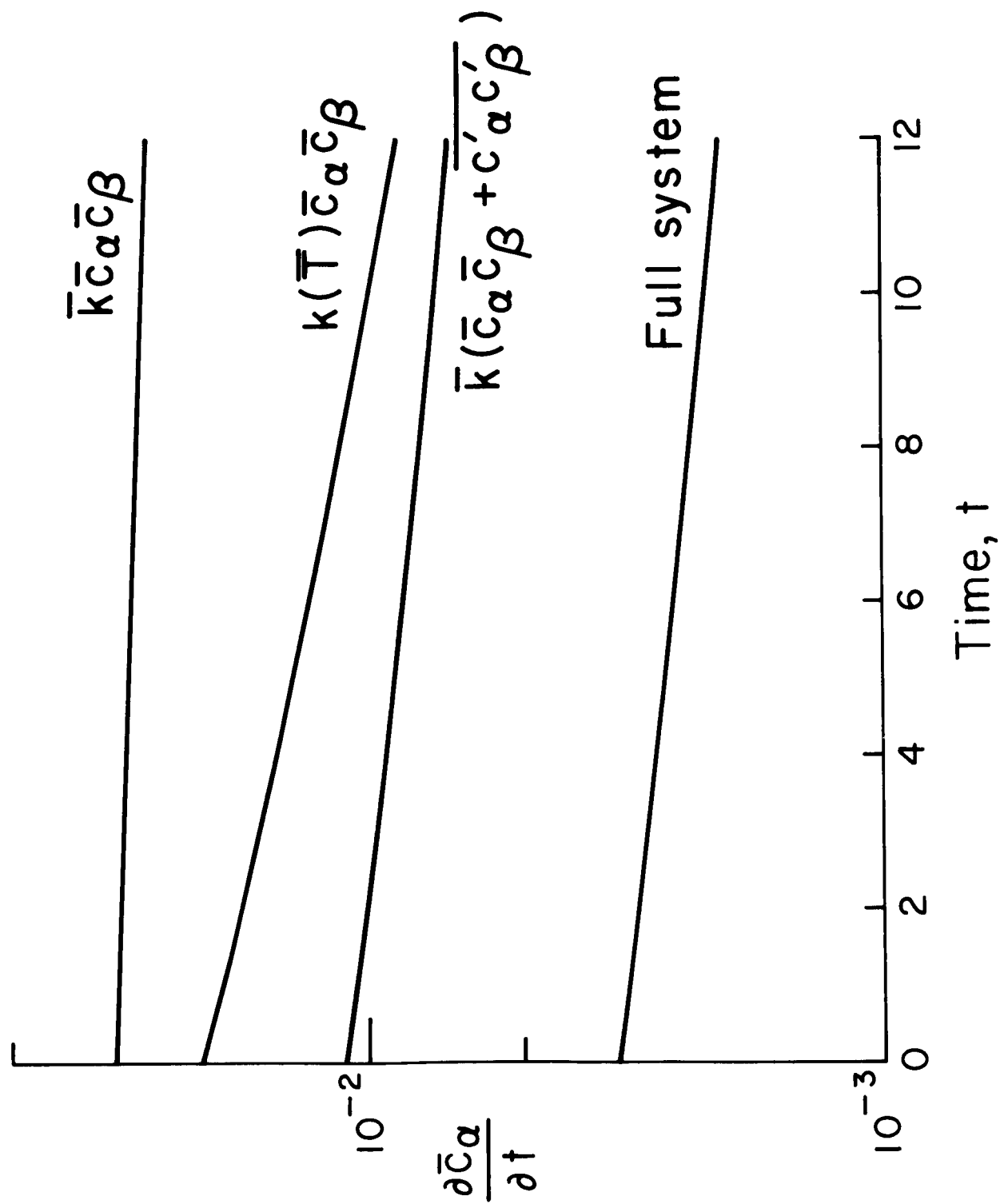


Figure 5. Component terms in the expression for rate of change of $\bar{\alpha}$

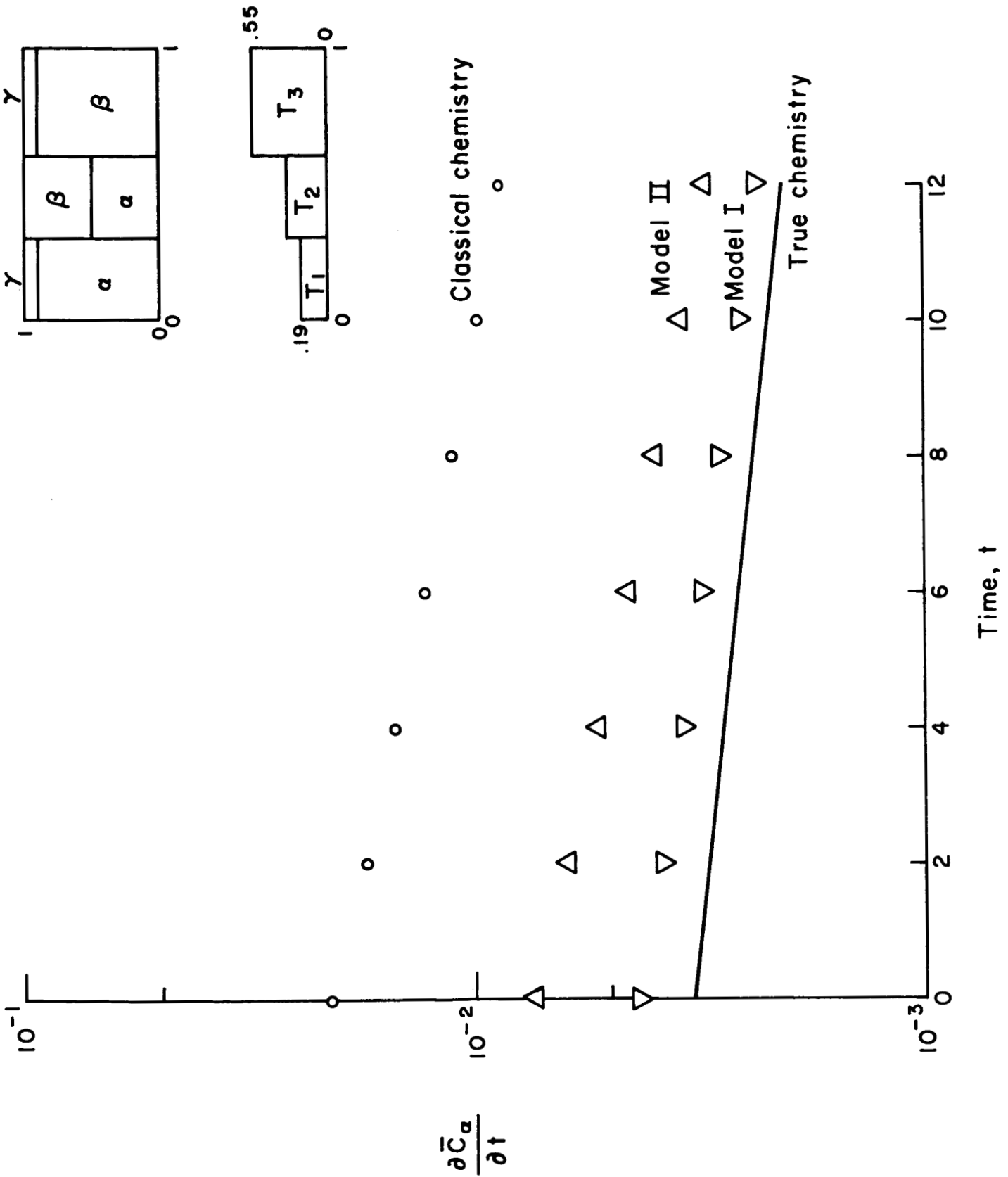


Figure 6. Base flow 1 to check correlation modeling; variable temperature cells

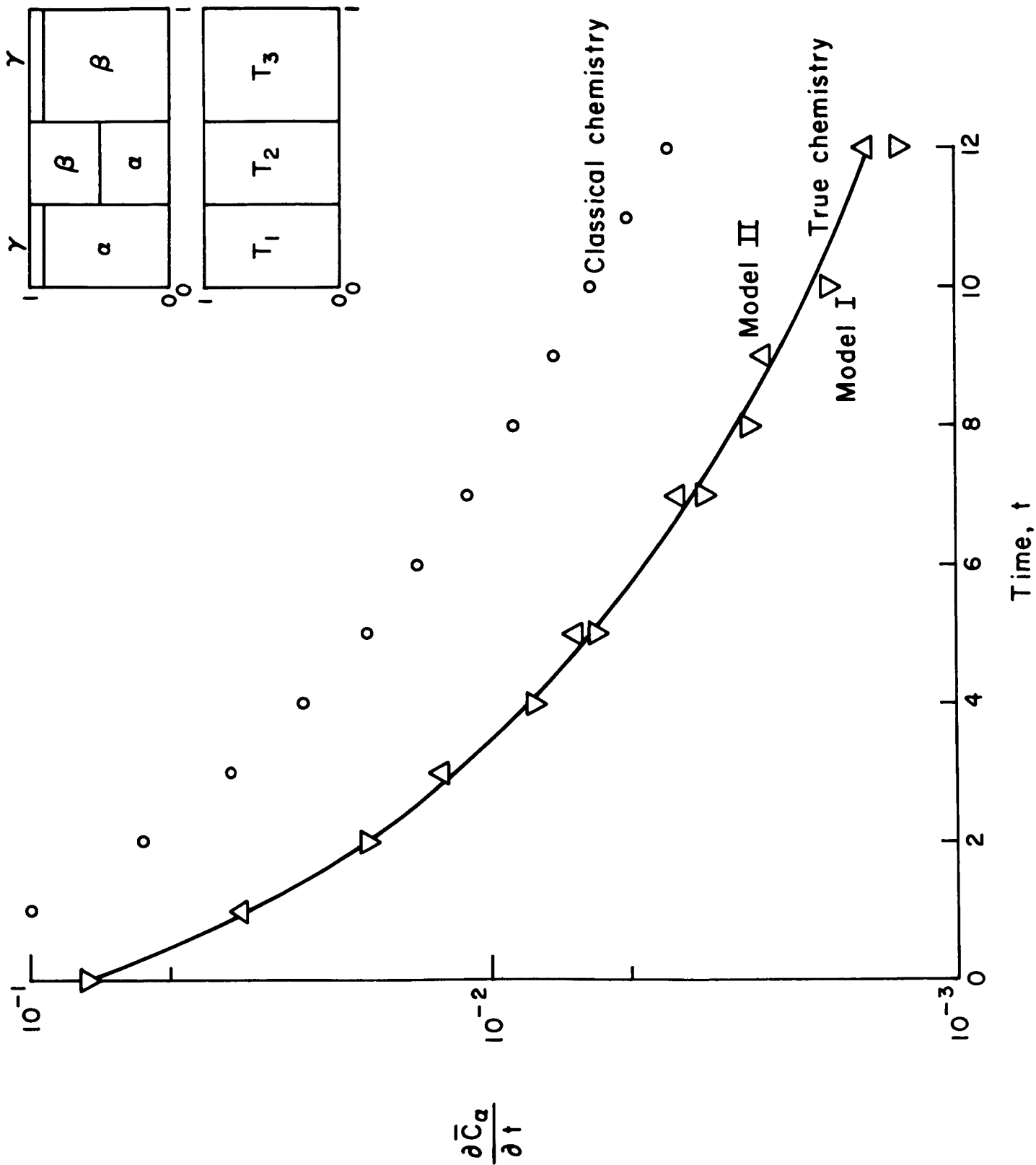


Figure 7. Base flow 1 to check correlation modeling; constant temperature cells

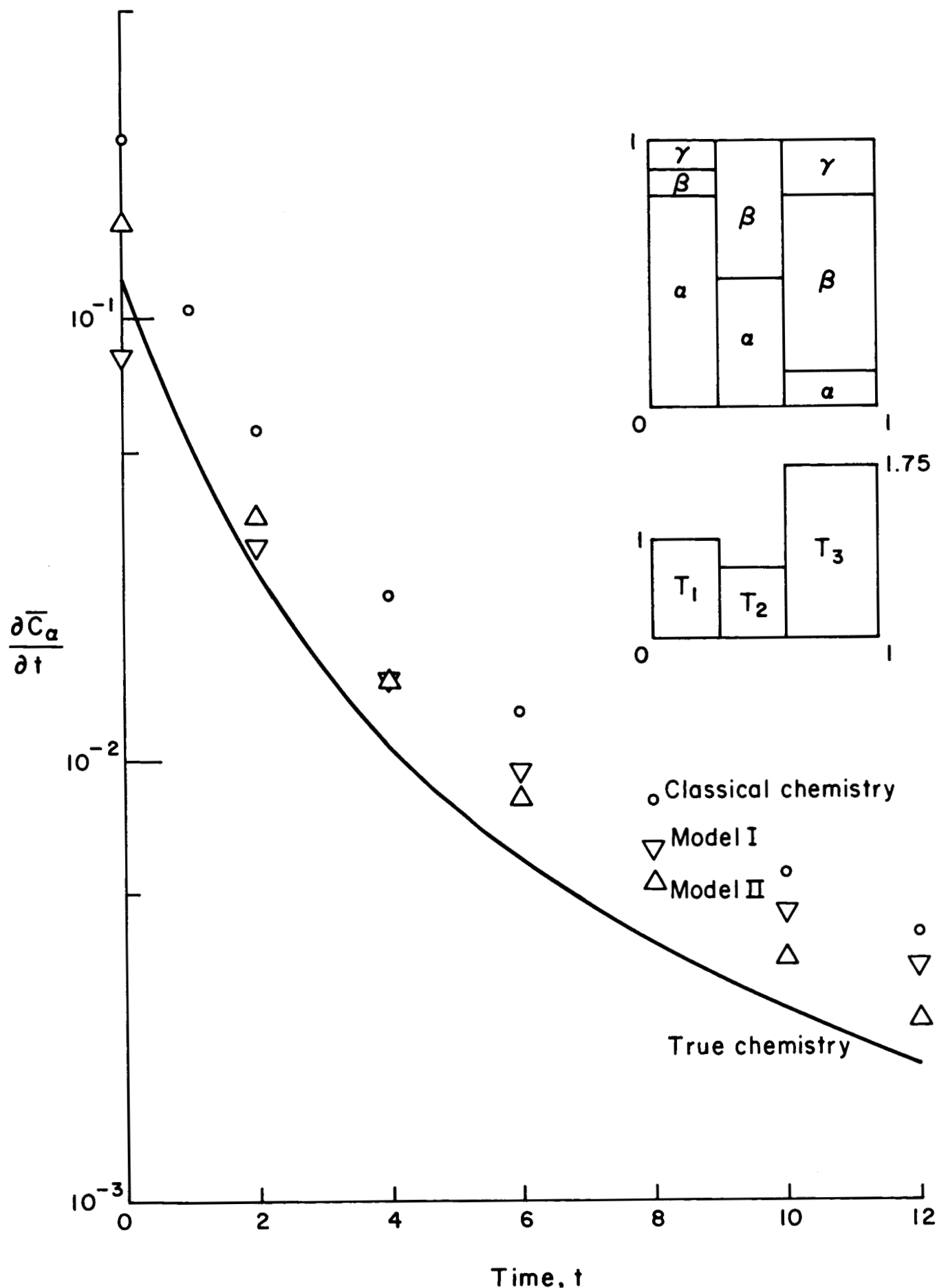


Figure 8. Base flow 2 to check correlation modeling; variable temperature cells

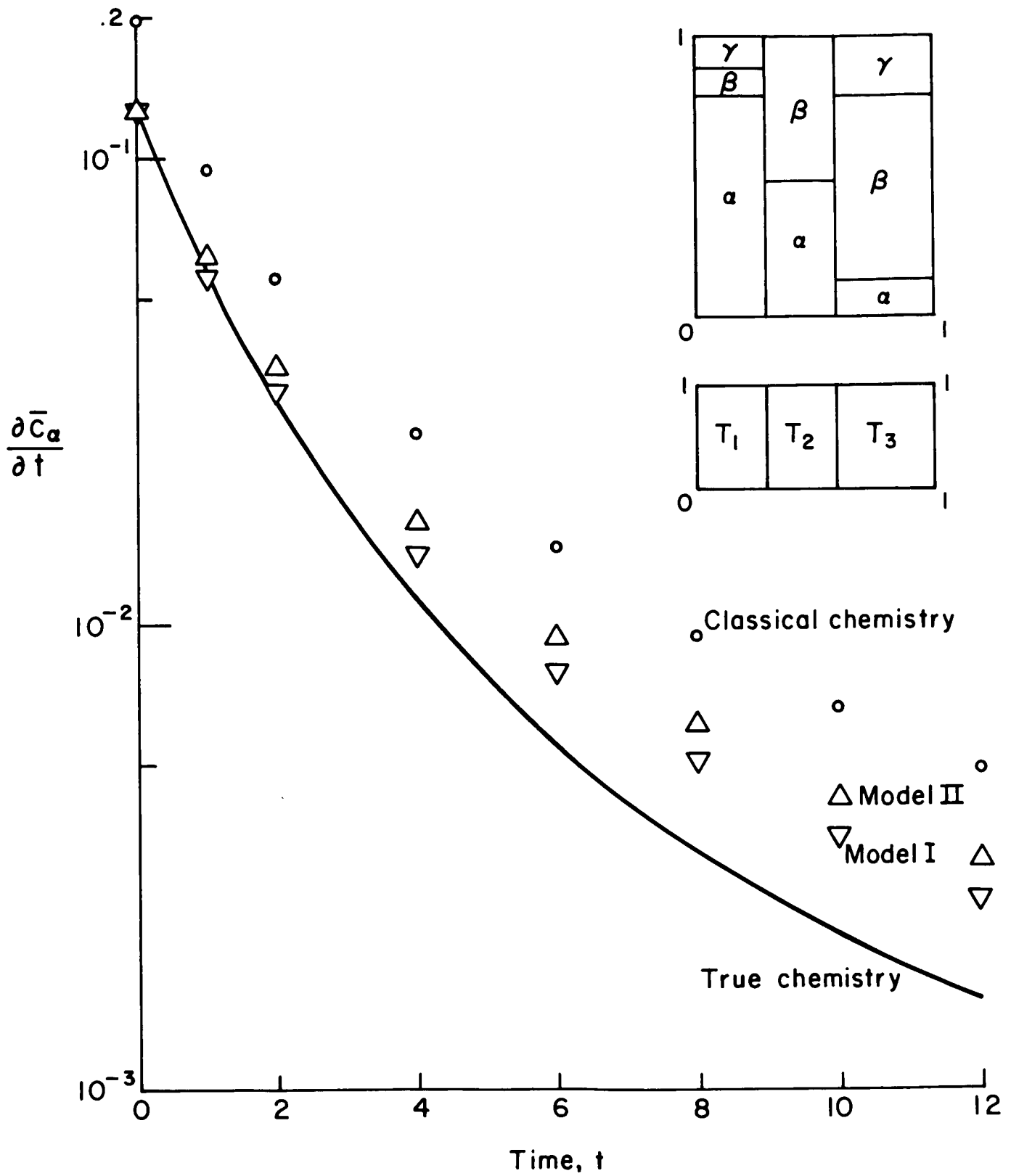


Figure 9. Base flow 2 to check correlation modeling; constant temperature cells

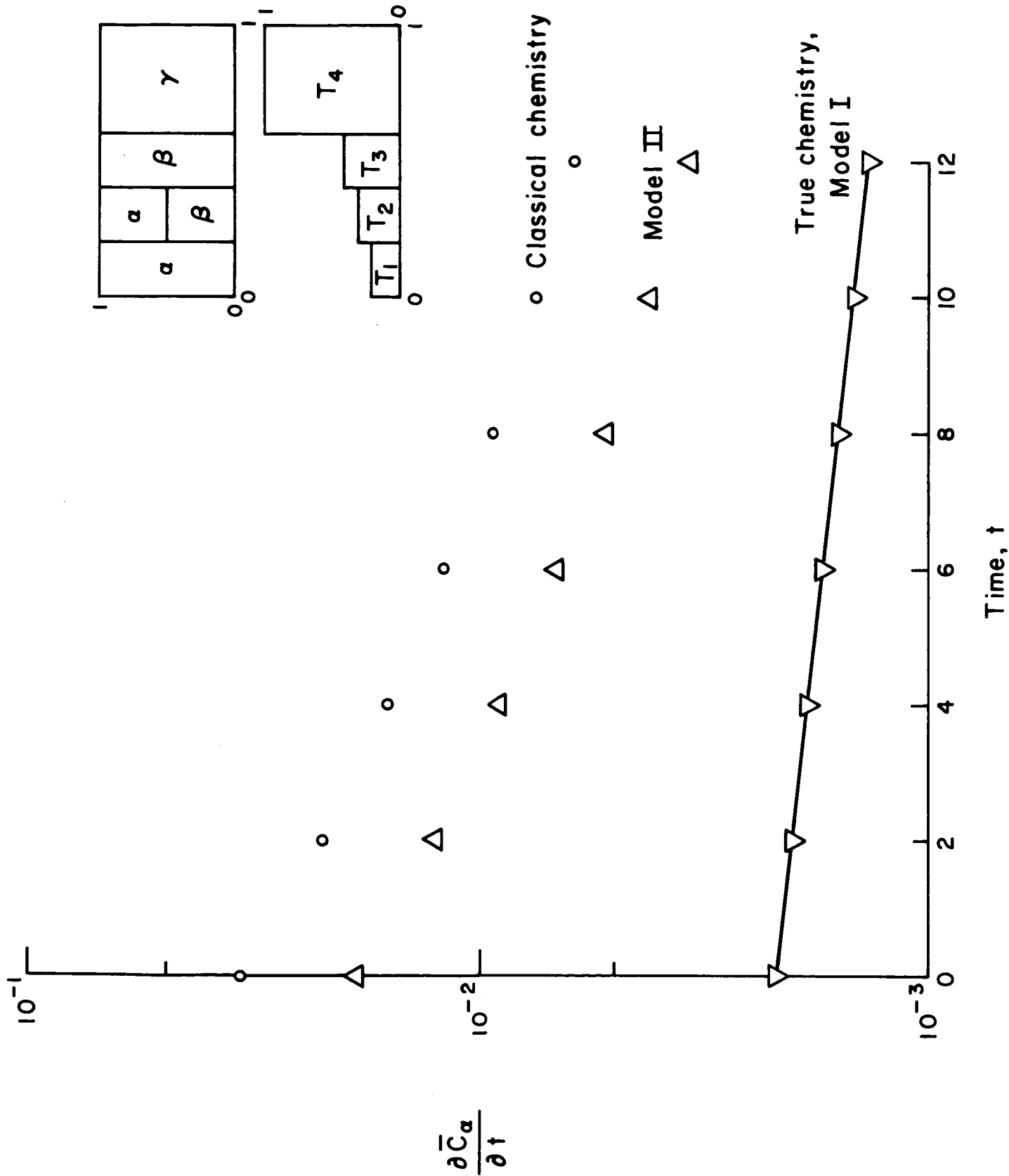


Figure 10. Base flow 3 to check correlation modeling; variable temperature cells

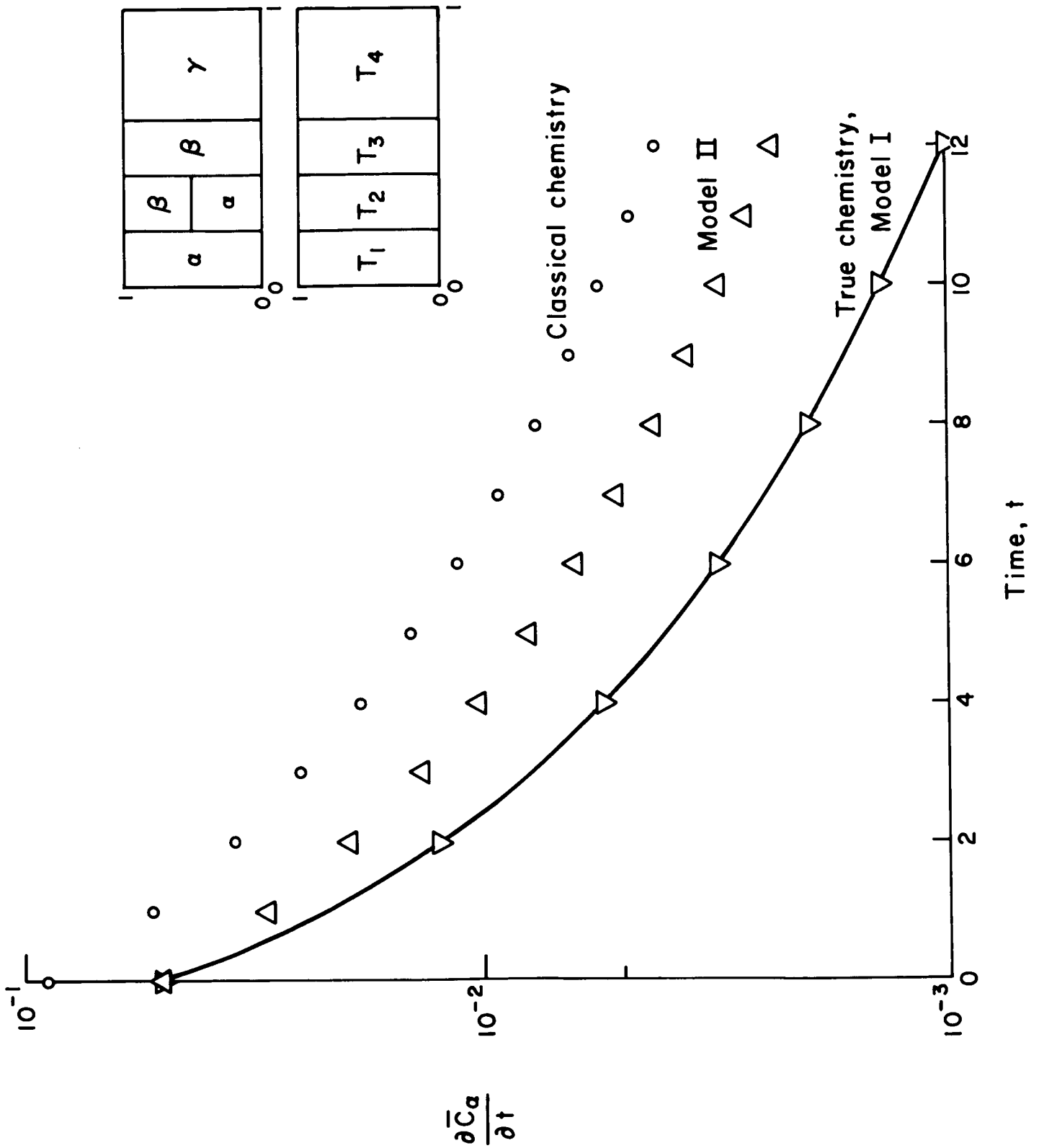


Figure 11. Base flow 3 to check correlation modeling; constant temperature cells

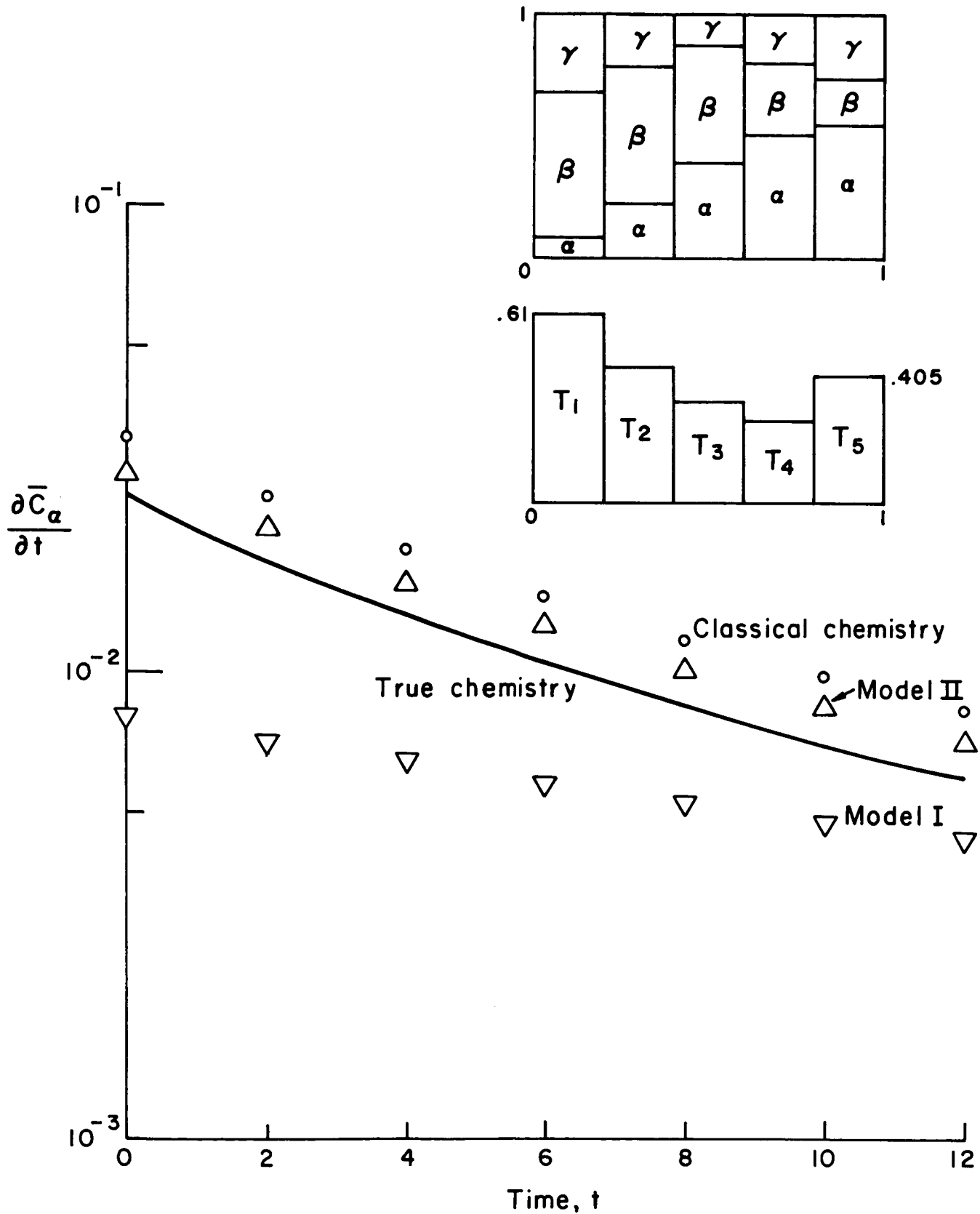


Figure 12. Base flow 4 to check correlation modeling; variable temperature cells

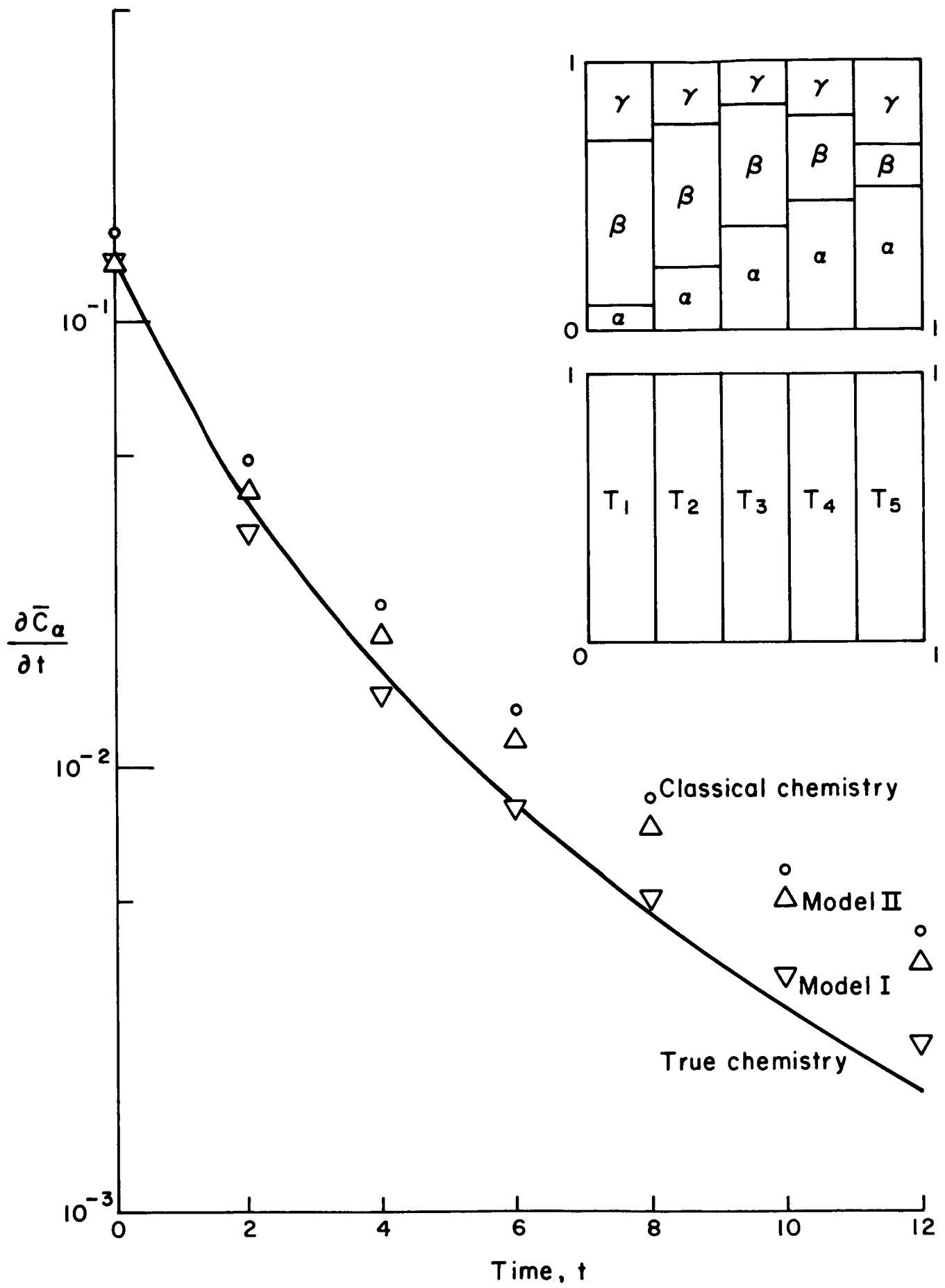


Figure 13. Base flow 4 to check correlation modeling; constant temperature cells

one or the other of the two models shows good agreement with the exact solution of the chemical kinetic equations. We have now developed a seven-cell model which incorporates the better features of the two models discussed above. This model, Model III, is described in the next section.

DESCRIPTION OF MODEL III

For this model, the typical eddy of extent unity in time is considered to have the following structure. For a time ϵ_1 the eddy contains only the species α . For a time ϵ_2 the eddy contains only the species β , and for time ϵ_3 the eddy contains only the species γ . For time equal to ϵ_4 , ϵ_5 , and ϵ_6 , the eddy is assumed to contain $1/2 \alpha$ and $1/2 \beta$, $1/2 \alpha$ and $1/2 \gamma$, and $1/2 \beta$ and $1/2 \gamma$ by mass, respectively, in a state of molecular mixedness. In addition, we assume that for a time

$$\epsilon_7 = \left(1 - \left| \frac{\overline{\alpha'\beta'}}{\overline{\alpha\beta}} \right| \right) \left(1 - \left| \frac{\overline{\alpha'\gamma'}}{\overline{\alpha\gamma}} \right| \right) \left(1 - \left| \frac{\overline{\beta'\gamma'}}{\overline{\beta\gamma}} \right| \right)$$

the eddy contains α , β and γ uniformly mixed and in proportion to the mean mass fractions $\overline{\alpha}$, $\overline{\beta}$, and $\overline{\gamma}$. Since the total extent of the eddy is unity,

$$\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4 + \epsilon_5 + \epsilon_6 = (1 - \epsilon_7)$$

$$= 1 - \left(1 - \left| \frac{\overline{\alpha'\beta'}}{\overline{\alpha\beta}} \right| \right) \left(1 - \left| \frac{\overline{\alpha'\gamma'}}{\overline{\alpha\gamma}} \right| \right) \left(1 - \left| \frac{\overline{\beta'\gamma'}}{\overline{\beta\gamma}} \right| \right)$$

Thus, the model has only five unknowns necessary to define the eddy which are determined by the five available equations for $\overline{\alpha}$, $\overline{\beta}$, $\overline{\alpha'\beta'}$, $\overline{\alpha'\gamma'}$, and $\overline{\beta'\gamma'}$. The temperature and the reaction rate distributions are set up in the same way as for Models I and II. Figure 14 illustrates the complete seven-cell model.

This model is currently being tested by comparison of model predictions to exact solutions of the chemical rate equations. Basically it is a combination of the two previous models, and we expect the results of these tests to be quite satisfactory. The model can be extended to the case of four species in a straightforward manner and collapses correctly to the cases of flows involving one or two species.

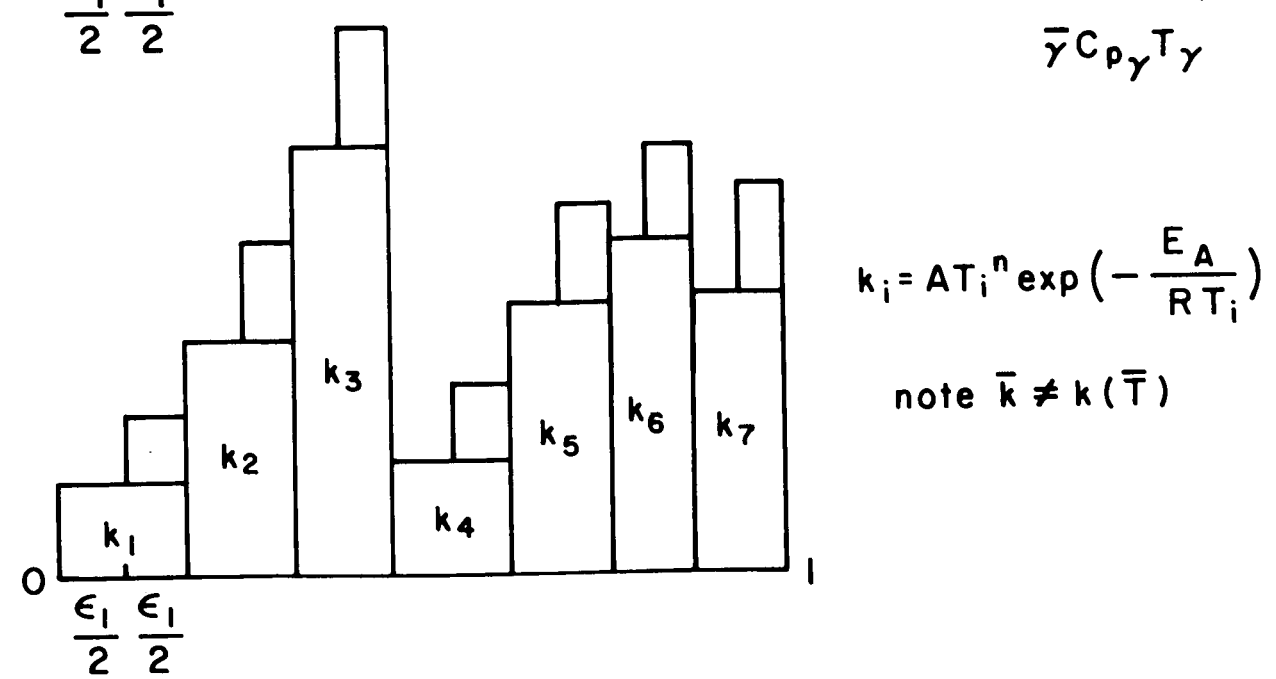
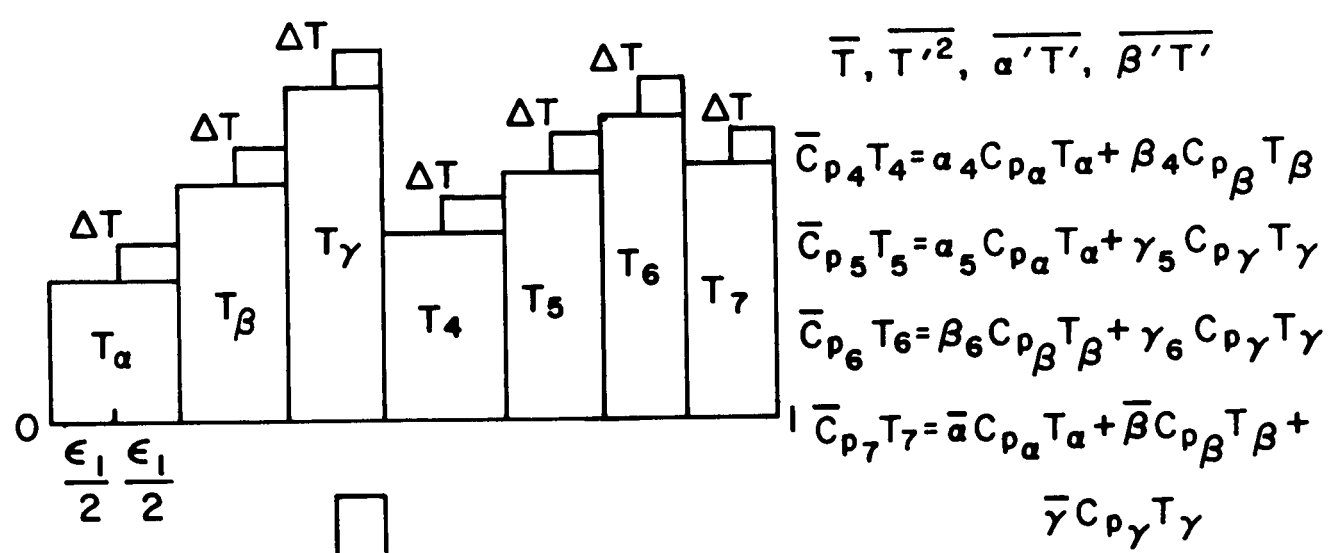
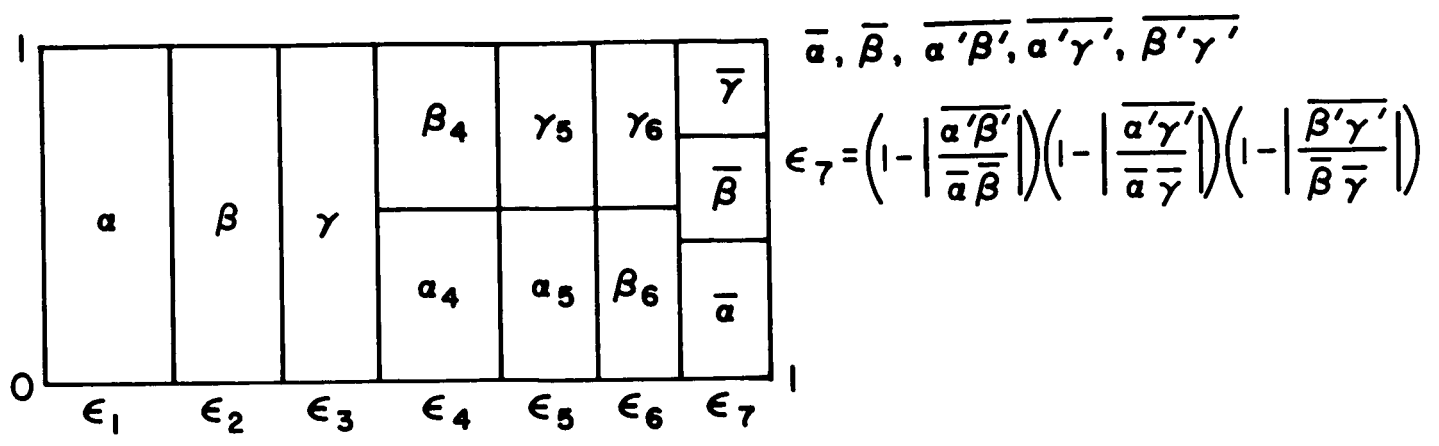


Figure 14. Seven-cell, three-species "typical eddy" model MODEL III

CONCLUSIONS

A "typical eddy" box model for the second-order closure of turbulent reacting flows has been developed. The model structure is quite general and is valid for an arbitrary number of species. Model predictions are significantly better than classical chemistry (involving only the means) computations and are in good agreement with exact solutions of the reaction rate equations for a number of assumed flow distributions.

The model enables calculation of any correlation of scalar fluctuations involving concentrations, temperatures, and reaction rates. It provides the capability of making a second-order closure computation of turbulent flames and other flows involving highly exothermic chemical reactions.

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