Numerical Approximating of Two Component Becker-Döring Equations

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Abstract: The process of collision between particles is a subject of interest in many fields of physics, astronomy, polymer physics, atmospheric physics and colloid chemistry. The time evolution of the cluster distribution has been described by an infinite system of ordinary differential equations. In this paper, for the two component model,truncated and two reduced models are defined and the numerical results show that the reduced models have a good accuracy and can be applied for studying the behavior of a bigger systems.

1 Introduction

Consider a system of identical particles that can collect into clusters, whose size is then an integer multiple of the base particle size. The cluster size distribution function $c_r(t)$ is a discrete function of cluster size r and represents the number of clusters of size r at time t per unit volume. The time evolution of the cluster distribution $c_r(t)$ has been described by the following infinite system of ordinary differential equations (*ODEs*) [1]

$$\dot{c}_r = \frac{1}{2}\sum_{k=1}^{r-1} J_{r-k,k} - \sum_{k=1}^{\infty} J_{r,k} \quad r = 1, 2, \cdots, \qquad (1)$$

where $J_{r,k} = a_{r,k}c_r c_k - b_{r,k}c_{r+k} = J_{k,r}$, and for $r = 1$ the first sum is omitted and called the *discrete coagulation-fragmentation* equations. $J_{r,k}$ is the net rate of converting the clusters with r-particles (r-clusters) to $(r+k)$-clusters, with non-negative symmetric constants $a_{r,k}$ and $b_{r,k}$ which determine the coagulation and fragmentation rates respectively.

Penrose, Carr and Hall [6] have generalized of the Becker-Döring model, using the kinetics of mixed micelle formation and defined the two component Becker-Döring model. In section 3, first, the two component Becker-Döring equations are derived and their main properties are described. Then for numerical approximation, the truncated model and two other reduced models are defined. The numerical results and discussion which are presented in the last sections, show that under some possible conditions on the kinetic coefficients and the densities, there is a metastable solution of the equations.

2 Two component Becker-Döring system

If two different types of particles are allowed to participate in the cluster coalescence, then the two component Becker-Döring dynamics is defined on the following hypothesis:

a) The number of particles of each type over all clusters is constant. (conserved quantities)

b) The clusters are distributed uniformly in space, therefore the expected number of particle clusters doesn't depend on the space variable and is only a function of time.

c) The cluster size distribution changes when clusters coagulate or fragment by gaining or losing monomers. (There are two types of monomers in the system.)

Let an (r,s)-particle cluster be a cluster with r particles of type I and s particles of type II, and let $c_{r,s}(t) \geq 0$ denote the expected number of (r,s)-particle clusters per unit volume at time t. There are two net rates for converting the clusters. $J_{r,s}$ is the rate at which (r,s)-clusters change to $(r+1,s)$-clusters, and $J'_{r,s}$ is the rate at which (r,s)-clusters alter to $(r,s+1)$-clusters. They are defined by

$$\begin{aligned} J_{r,s} &= a_{r,s}c_{r,s}c_{1,0} - b_{r+1,s}c_{r+1,s}, \\ J'_{r,s} &= a'_{r,s}c_{r,s}c_{0,1} - b'_{r,s+1}c_{r,s+1}, \end{aligned} \qquad (2)$$

where $a_{r,s}, b_{r,s}$ are the kinetic coefficients (coagulation, fragmentation rates) for the particle of type I and $a'_{r,s}, b'_{r,s}$ are the coagulation, fragmentation rates of particles of type II. All coefficients are non-negative constants with $b_{1,0} = 0$, $b'_{0,1} = 0$. The two component Becker-Döring dynamics can be formulated as

$$\begin{aligned} \dot{c}_{r,s} &= J_{r-1,s} + J'_{r,s-1} - J_{r,s} - J'_{r,s} && r \geq 1, s \geq 1, \\ \dot{c}_{r,0} &= J_{r-1,0} - J_{r,0} - J'_{r,0} && r \geq 2, \\ \dot{c}_{0,s} &= J'_{0,s-1} - J_{0,s} - J'_{0,s} && s \geq 2. \end{aligned} \qquad (3)$$

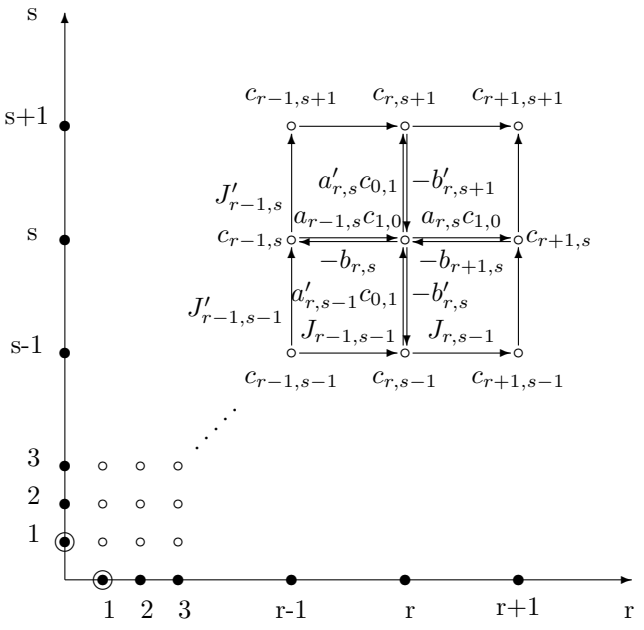

Figure 1: The schematic process of the two component Becker-Döring system.

Conservation of the total number of particles of each species in the system leads to the following equations for the monomer concentration:

$$\dot{c}_{1,0} = -J_{1,0} - J'_{1,0} - \sum_{(r,s)\in I_f} J_{r,s}$$
$$\dot{c}_{0,1} = -J_{0,1} - J'_{0,1} - \sum_{(r,s)\in I_f} J'_{r,s} \qquad (4)$$

where

$$I_f = \{(r,s), \quad r = 0,1,2,\cdots, \quad s = 0,1,2,\cdots\} - \{(0,0)\}.$$

Figure 1 shows a schematic diagram of the (r,s)-clusters gaining and losing monomers at the specified rates. The monomers appear at the location $(0,1)$ and $(1,0)$ on the diagram.

There is not much known about this system. Our references for the theory of the two component Becker-Döring system are [6] and [8]. Its behavior is more complex than the one component system. In this paper, as a first numerical experiment on this system, the truncated model and two reduced models will be described and the numerical results will be presented. The last section includes a discussion and some remarkable points of our experience.

2.1 Truncated Model

The two component Becker-Döring system is formulated as an infinite system of differential equations, and so for numerical approximation, the system has to be truncated. If n_r , n_s are the largest number of particles of types I and II which can be collected in one cluster, then the size of the finite dimensional model is $(n_r+1)(n_s+1)-1$. With this assumption the conversion rates

$$J_{r,s} = 0 \ , \ J'_{r,s} = 0, \quad \text{if } \ r \geq n_r \ \text{ or } \ s \geq n_s. \qquad (5)$$

In the truncated model, all indices of $c_{r,s}$ can be considered as a point (r,s) on the rectangle with vertices $(n_r,0),(0,n_s),(n_r,n_s)$ and (0, 0), i.e. $(r,s) \in I_t$ where

$$I_t = \{(r,s), \quad r = 0,1,\cdots, \ \ n_r \ \ , s = 0,1,\cdots,n_s\} - \{(0,0)\}.$$

All points inside the rectangle can gain or lose each type of monomer but there are restrictions on how the clusters on its boundary coagulate and fragment. For example $(0,n_s)$-clusters can not coagulate with $(0,1)$-clusters, since $J'_{0,n_s} = 0$. With the above description, the truncated model can be formulated as follows :

a) For (r,s)-clusters with (r,s) inside the rectangle

$$\begin{aligned} \dot{c}_{r,s} &= J_{r-1,s} + J'_{r,s-1} - J_{r,s} - J'_{r,s} \qquad (6)\\ r &= 1,2,\cdots,n_r-1 \quad , \quad s = 1,2,\cdots,n_s-1 \end{aligned}$$

b) (r,s) on the rectangle sides

$$\begin{aligned} \dot{c}_{r,0} &= J_{r-1,0} - J_{r,0} - J'_{r,0} \\ & \qquad r = 2,3,\cdots,n_r-1 \\ \dot{c}_{0,s} &= J'_{0,s-1} - J_{0,s} - J'_{0,s} \qquad (7)\\ & \qquad s = 2,3,\cdots,n_s-1 \\ \dot{c}_{n_r,s} &= J_{n_r-1,s} + J'_{n_r,s-1} - J'_{n_r,s} \\ & \qquad s = 1,2,\cdots,n_s-1 \\ \dot{c}_{r,n_s} &= J_{r-1,n_s} + J'_{r,n_s-1} - J_{r,n_s} \\ & \qquad r = 1,2,\cdots,n_r-1 \end{aligned}$$

c) For the rectangle vertices

$$\begin{aligned} \dot{c}_{n_r,0} &= J_{n_r-1,0} - J'_{n_r,0} \\ \dot{c}_{0,n_s} &= J'_{0,n_s-1} - J_{0,n_s} \qquad (8)\\ \dot{c}_{n_r,n_s} &= J_{n_r-1,n_s} + J'_{n_r,n_s-1} \end{aligned}$$

d) For the monomers

$$\begin{aligned} \dot{c}_{1,0} &= -J_{1,0} - J'_{1,0} - \sum_{(r,s)\in I_t} J_{r,s} \qquad (9)\\ \dot{c}_{0,1} &= -J_{0,1} - J'_{0,1} - \sum_{(r,s)\in I_t} J'_{r,s}. \end{aligned}$$

The densities of this truncated system are defined by

$$\rho_{\mathrm{I}} = \sum_{(r,s)\in I_t} r c_{r,s} \quad , \quad \rho_{\mathrm{II}} = \sum_{(r,s)\in I_t} s c_{r,s} \qquad (10)$$

with the sum reduced from I_f to I_t. It can easily be proved that ρ_{I} and ρ_{II} are independent of time in the full and truncated model.

It is not difficult to prove that the equations (9) and (10) are equivalent. We can then apply the density conservation formulae instead of the monomer rate equations (9) in our numerical algorithm.

We will present results with two different kinetic sets of coefficients as follows:

a)

$$\begin{aligned} a_{r,s} &= 1 \quad , \quad a'_{r,s} = 1 \\ Q_{r,s} &= \exp[-a(r-1)^{2/3} - b(s-1)^{2/3}] \end{aligned} \tag{11}$$

b)

$$\begin{aligned} a_{r,s} &= 1 \quad , \quad a'_{r,s} = 1 \\ Q_{r,s} &= \exp[-a(r+s-2)^{2/3}]. \end{aligned} \tag{12}$$

In the both cases the fragmentation coefficients are

$$b_{r,s} = \frac{a_{r-1,s} Q_{r-1,s}}{Q_{r,s}} \quad , \quad b'_{r,s} = \frac{a'_{r,s-1} Q_{r,s-1}}{Q_{r,s}}.$$

and the system is initialized with monomers,that means

$$\begin{aligned} c_{0,1}(0) &= \rho_{\mathrm{II}} \\ c_{1,0}(0) &= \rho_{\mathrm{I}} \\ c_{r,s}(0) &= 0 \quad \text{if} \quad r+s > 1. \end{aligned} \tag{13}$$

The system we consider is the truncated version with *ODE*s (6), (7), (8) and the density conservation equations (10). This is a differential algebraic equation (*DAE*) with two algebraic equations. For the numerical solution, we write the two dimensional array $c_{r,s}$ as a vector using the formula:

$$y_{r(n_s+1)+s} = c_{r,s} \qquad \text{where} \qquad (r,s) \in I_t.$$

The variables are ordered from $y_1 = c_{0,1}$ to $y_{(n_r+1)(n_s+1)-1} = c_{n_r,n_s}$.

The *DAE* system can then be written as

$$\left\{ \begin{array}{ll} \dot{\underline{y}} = & \underline{f}(\underline{y}), \\ \underline{0} = & \underline{g}(\underline{y}). \end{array} \right. \tag{14}$$

It is a stiff system and is integrated with the backward difference formula

$$\left\{ \begin{array}{ll} \underline{y}^{k+1} - \underline{y}^k - h^{k+1} & \underline{f}(\underline{y}^{k+1}) = \quad 0, \\ & \underline{g}(\underline{y}^{k+1}) = \quad 0. \end{array} \right. \tag{15}$$

To solve the above nonlinear algebraic system for $\underline{y}^{k+1}$ by the Newton method, we need to calculate the Jacobian. The Jacobian is a very big matrix, but it is sparse and has a regular structure [7, 3].

2.2 Reduced Models

For the two component model, the system size is even more of a problem than for the one component system. For example even if we choose $n_r = n_s = 100$ for the largest particle numbers of each type in one cluster, then the truncated model is formulated with 10200 equations and the Jacobian is a 10200×10200 matrix with 71000 non-zero elements. This shows that running the truncated model even for a small size of each component needs a lot of memory and work. In this section, using our experience with the one component Becker-Döring , two reduced models are defined.

2.2.1 Constant Fluxes

assume the fluxes for each type of particle are constant, i.e.

$$\begin{aligned} J_{r,s} &= \hat{J}_s \qquad s = 1, 2, \cdots, n_s - 1 \\ J'_{r,s} &= \hat{J}'_r \qquad r = 1, 2, \cdots, n_r - 1. \end{aligned} \tag{16}$$

Now using the definition of $J_{r,s}$ and $Q_{r,s}$ we have

$$\begin{aligned} \frac{J_{k,s}}{a_{k,s} Q_{k,s} c_{1,0}^{k+1}} &= \frac{c_{k,s}}{Q_{k,s} c_{1,0}^{k}} - \frac{b_{k+1,s} c_{k+1,s}}{a_{k,s} Q_{k,s} c_{1,0}^{k+1}} \\ &= \frac{c_{k,s}}{Q_{k,s} c_{1,0}^{k}} - \frac{c_{k+1,s}}{Q_{k+1,s} c_{1,0}^{k+1}}, \end{aligned}$$

and similarly

$$\frac{J'_{r,k}}{a'_{r,k} Q_{r,k} c_{0,1}^{k+1}} = \frac{c_{r,k}}{Q_{r,k} c_{0,1}^{k}} - \frac{c_{r,k+1}}{Q_{r,k+1} c_{0,1}^{k+1}}.$$

The right hand side terms are two successive expressions with respect to k, therefore the following identities can be obtained

$$\sum_{k=\ell}^{m} \frac{J_{k,s}}{a_{k,s} Q_{k,s} c_{1,0}^{k+1}} = \frac{c_{\ell,s}}{Q_{\ell,s} c_{1,0}^{\ell}} - \frac{c_{m+1,s}}{Q_{m+1,s} c_{1,0}^{m+1}} \tag{17}$$

$$\sum_{k=\ell}^{m} \frac{J'_{r,k}}{a'_{r,k} Q_{r,k} c_{0,1}^{k+1}} = \frac{c_{r,\ell}}{Q_{r,\ell} c_{0,1}^{\ell}} - \frac{c_{r,m+1}}{Q_{r,m+1} c_{0,1}^{m+1}} \tag{18}$$

From (16) and (17) with $\ell = 0$ and $m = r - 1$ for fixed s,

$$c_{r,s} = Q_{r,s} c_{1,0}^{r} \left(\frac{c_{0,s}}{Q_{0,s}} - \hat{J}_s \sum_{k=0}^{r-1} 1/(a_{k,s} Q_{k,s} c_{1,0}^{k+1}) \right) \quad r = 1, 2, \cdots, n_r - 1 \tag{19}$$

where $\hat{J}_s$ is obtained from (17) with $l = 0$ and $m = n_r - 1$, i.e.

$$\hat{J}_s = \frac{\frac{c_{0,s}}{Q_{0,s}} - \frac{c_{n_r,s}}{Q_{n_r,s} c_{1,0}^{n_r}}}{\sum_{k=0}^{n_r-1} 1/(a_{k,s} Q_{k,s} c_{1,0}^{k+1})}.$$

Similarly for all values of s and fixed r , from (18)

$$c_{r,s} = Q_{r,s} c_{0,1}^{s} \left(\frac{c_{r,0}}{Q_{r,0}} - \hat{J}'_r \sum_{k=0}^{s-1} 1/(a'_{r,k} Q_{r,k} c_{0,1}^{k+1}) \right) \quad s = 1, 2, \cdots, n_s - 1 \tag{20}$$

where

$$\hat{J}'_r = \frac{\frac{c_{r,0}}{Q_{r,0}} - \frac{c_{r,n_s}}{Q_{r,n_s} c_{0,1}^{n_s}}}{\sum_{k=0}^{n_s-1} 1/(a'_{r,k} Q_{r,k} c_{0,1}^{k+1})}.$$

With the above procedure (19) and (20) give two different values for $c_{r,s}$, and so we define $c_{r,s}$ to be the weighted average

$$c_{r,s} = \frac{r c_{r,s}^{(19)} + s c_{r,s}^{(20)}}{r+s}, \tag{21}$$

where $c^{(19)}_{r,s}$ is the $c_{r,s}$ in (19).

Therefore using assumption (16), $(n_r+1)(n_s+1)-1$ equations in the truncated model can be reduced to $2(n_r+n_s)-1$ equations depending on the variables on the boundary area, as follows :

$$\begin{aligned}
\rho_{\rm I} &= \sum_{(r,s)\in I_t} r c_{r,s} \quad , \quad \rho_{\rm II} = \sum_{(r,s)\in I_t} s c_{r,s} \\
\dot{c}_{r,0} &= J_{r-1,0} - J_{r,0} - \hat{J}'_r \qquad r = 2,3,\cdots,n_r-1 \\
\dot{c}_{0,s} &= J'_{0,s-1} - J'_{0,s} - \hat{J}_s \qquad s = 2,3,\cdots,n_s-1 \\
\dot{c}_{n_r,s} &= J'_{n_r,s-1} - J'_{n_r,s} + \hat{J}_s \qquad s = 1,2,\cdots,n_s-1 \\
\dot{c}_{r,n_s} &= J_{r-1,n_s} - J_{r,n_s} + \hat{J}'_r \qquad r = 1,2,\cdots,n_r-1 \\
\dot{c}_{0,n_s} &= J'_{0,n_s-1} - J_{0,n_s} \\
\dot{c}_{n_r,0} &= J_{n_r-1,0} - J'_{n_r,0} \\
\dot{c}_{n_r,n_s} &= J_{n_r-1,n_s} + J'_{n_r,n_s-1}
\end{aligned}$$

where I_t is the index set for the truncated model.

The balances of the converting rates for all $c_{r,s}$ not on the boundary are zero and so the solution of the following in the interior algebraic equations gives the values of $c_{r,s}$

$$\begin{aligned}
& J_{r-1,s} - J_{r,s} + J'_{r,s-1} - J'_{r,s} = 0 \qquad (22) \\
& r = 1,2,\cdots,n_r-1 \quad , \quad s = 1,2,\cdots,n_s-1
\end{aligned}$$

The above system can be written in matrix form, $AG = B$, where A is a block penta-diagonal matrix.

$$A = \begin{bmatrix}
A_1 & U_1 & & & & \\
L_1 & A_2 & U_2 & & & \\
 & L_3 & A_3 & U_3 & & \\
 & & & \ddots & U_{n_r-1} & \\
 & & & L_{n_r-2} & A_{n_r-1}
\end{bmatrix},$$

$$\begin{aligned}
G &= [\ G_1 \quad G_2 \quad \cdots \quad G_{n_r-1}\ ]^T \\
B &= [\ B_1 \quad B_2 \quad \cdots \quad B_{n_r-1}\ ]^T
\end{aligned}$$

where A_i, L_i and U_i are $(n_s-1)\times(n_s-1)$ matrices,

$$A_i = \begin{bmatrix}
-\Delta_{i,1} & b'_{i,2} & & & \\
a'_{i,1}c_{0,1} & -\Delta_{i,2} & b'_{i,3} & & \\
 & & \ddots & & b'_{i,n_s-1} \\
 & & & a'_{i,n_s-2}c_{0,1} & -\Delta_{i,n_s-1}
\end{bmatrix}$$

$$L_i = c_{1,0}\begin{bmatrix}
a_{i,1} & & & \\
 & a_{i,2} & & \\
 & & \ddots & \\
 & & & a_{i,n_s-1}
\end{bmatrix},$$

$$U_i = \begin{bmatrix}
b_{i+1,1} & & & \\
 & b_{i+1,2} & & \\
 & & \ddots & \\
 & & & b_{i+1,n_s-1}
\end{bmatrix}$$

with

$$\Delta_{i,j} = b_{i,j} + a_{i,j}c_{1,0} + b'_{i,j} + a'_{i,j}c_{0,1},$$

and G_i, B_i are $(n_s-1)\times 1$ vectors

$$\begin{aligned}
G_i &= [\ c_{i,1} \quad c_{i,2} \quad c_{i,3} \quad \cdots \quad c_{i,n_s-1}\ ]^T \\
B_i &= [\ -a'_{i,0}c_{0,1}c_{i,0} \quad 0 \quad 0 \quad \cdots \quad 0 \quad b'_{i,n_s}c_{i,n_s}\ ]^T, \\
&\qquad\qquad i = 1,2,\cdots,n_r-1 \\
B_1 &= B_1 + c_{1,0}[-a_{0,1}c_{0,1}, -a_{0,2}c_{0,2}, \cdots, \\
&\qquad\qquad -a_{0,n_s-1}c_{0,n_s-1}]^T \\
B_{n_r-1} &= B_{n_r-1} + [-b_{n_r,1}c_{n_r,1}, -b_{n_r,2}c_{n_r,2}, \\
&\qquad\qquad \cdots, -b_{n_r,n_s-1}c_{n_r,n_s-1}]^T
\end{aligned}$$

We have solved this large system using direct block LU factorization.

2.2.2 Piecewise Constant Fluxes

Let us select a subset of the nodes in the r and s components

$$\begin{aligned}
&\{n_{r_i}\}_{i=0}^{k} \subseteq \{0,1,2,\cdots,n_r\} \\
&\{n_{s_j}\}_{j=0}^{\ell} \subseteq \{0,1,2,\cdots,n_s\}
\end{aligned}$$

then the index set of nodes is

$$\begin{aligned}
I_r &= \{(n_{r_i}, n_{s_j})\ ,\ i = 0,1,2,\cdots,k\ , \\
&\qquad j = 0,1,2,\cdots,\ell\} - \{(0,0)\} \subseteq I_t
\end{aligned}$$

with the following restrictions :

$$\begin{aligned}
n_{r_0} &= n_{s_0} = 0, \qquad n_{r_k} = n_r \\
n_{r_1} &= n_{s_1} = 1, \qquad n_{s_\ell} = n_s.
\end{aligned}$$

Now assume that the converting rates are piecewise constant as follows:

$$\begin{aligned}
J_{r,s} &= \hat{J}_{i,s} \quad \text{if} \quad n_{r_i} < r < n_{r_{i+1}}, \\
J'_{r,s} &= \hat{J}'_{r,j} \quad \text{if} \quad n_{s_j} < s < n_{s_{j+1}}.
\end{aligned}$$

Thus the domain $(r,s) \in I_t$ in the truncated model (rectangular region) is divided into $\ell \times k$ blocks or sub-rectangles and both fluxes are constant over each sub-rectangle. The $(n_r+1)\times(n_s+1)-1$ equations in the truncated model reduce to $n_r(\ell+1)+n_s(k+1)-\ell k$ equations in this model.

For formulating this piecewise constant fluxes model, we need to define the following sets:

$$\begin{aligned}
I_{r_1} &= \{n_{r_i}, i = 1,2,\cdots,k-1\} \\
I_{r_2} &= \{1,2,\cdots,n_r-1\} - I_{r_1} \\
I_{s_1} &= \{n_{s_j}, j = 1,2,\cdots,\ell-1\} \\
I_{s_2} &= \{1,2,\cdots,n_s-1\} - I_{s_1}
\end{aligned}$$

then the piecewise constant fluxes version of the two component Becker-Döring model is :

$$\dot{c}_{r,s} = J_{r-1,s} - J_{r,s} + J'_{r,s-1} - J'_{r,s} \quad (r,s) \in I_{r_1} \times I_{s_1}$$

$$
\begin{aligned}
\dot{c}_{n_{r_i},s} &= \hat{J}_{i-1,s} - \hat{J}_{i,s} + J'_{n_{r_i},s-1} - J'_{n_{r_i},s} \\
&\qquad i = 1, 2, \cdots, k-1, s \in I_{s_2} \\
\dot{c}_{r,n_{s_j}} &= \hat{J}'_{r,j-1} - \hat{J}'_{r,j} + J_{r-1,n_{s_j}} - J_{r,n_{s_j}} \\
&\qquad j = 1, 2, \cdots, \ell-1, r \in I_{r_2} \\
\dot{c}_{0,s} &= J'_{0,s-1} - J'_{0,s} - J_{0,s} \qquad s \in I_{s_1} - \{1\} \\
\dot{c}_{0,s} &= J'_{0,s-1} - J'_{0,s} - \hat{J}_{0,s} \qquad s \in I_{s_2} \\
\dot{c}_{r,0} &= J_{r-1,0} - J_{r,0} - J'_{r,0} \qquad r \in I_{r_1} - \{1\} \\
\dot{c}_{r,0} &= J_{r-1,0} - J_{r,0} - \hat{J}'_{r,0} \qquad r \in I_{r_2} \\
\dot{c}_{r,n_s} &= J_{r-1,n_s} - J_{r,n_s} + J'_{r,n_s-1} \qquad r \in I_{r_1} \\
\dot{c}_{r,n_s} &= J_{r-1,n_s} - J_{r,n_s} + \hat{J}'_{r,\ell-1} \qquad r \in I_{r_2} \\
\dot{c}_{n_r,s} &= J'_{n_r,s-1} - J'_{n_r,s} + J_{n_r-1,s} \qquad s \in I_{s_1} \\
\dot{c}_{n_r,s} &= J'_{n_r,s-1} - J'_{n_r,s} + \hat{J}_{k-1,s} \qquad s \in I_{s_2} \\
\dot{c}_{0,n_s} &= J'_{0,n_s-1} - J_{0,n_s} \\
\dot{c}_{n_r,0} &= J_{n_r-1,0} - J'_{n_r,0} \\
\dot{c}_{n_r,n_s} &= J_{n_r-1,n_s} + J'_{n_r,n_s-1}
\end{aligned}
$$

with the monomer rate equations

$$
\begin{aligned}
\dot{c}_{1,0} &= -J_{1,0} - J'_{1,0} - \sum_{(r,s)\in I_t} J_{r,s}, \\
\dot{c}_{0,1} &= -J_{0,1} - J'_{0,1} - \sum_{(r,s)\in I_t} J'_{r,s}.
\end{aligned}
$$

The equivalent densities conservation formulae are

$$
\rho_{\mathrm{I}} = \sum_{(r,s)\in I_t} r c_{r,s} \qquad , \qquad \rho_{\mathrm{II}} = \sum_{(r,s)\in I_t} s c_{r,s}.
$$

We are forced to calculate all $c_{r,s}$ at each time step no matter which formulae we use for the monomers. Following (19) and (20) , we solve the following algebraic system over each sub-rectangle.

$$
J_{r-1,s} - J_{r,s} = 0 \ , \ J'_{r,s-1} - J'_{r,s} = 0 \quad (r,s) \in I_t - I_r \ (23)
$$

Equations in rows or columns form tridiagonal algebraic sub-systems.

Figure 2 shows the monomer concentrations for the three models of two component Becker-Döring system with the kinetic coefficients in (11) and $a = b = 10$. The system size is 30×30 and the densities are $\rho_{\mathrm{I}} = \rho_{\mathrm{II}} = 350$.

For our models, $n_r = n_s$ so the system solutions can be considered as a square matrix and the system is symmetric because of the definition of the kinetic coefficients and equal system densities. Therefore the 1-norm and ∞-norm are the same. The accuracy of the reduced models can be computed by comparing with the truncated model. Two errors will be considered :

$$
||c^{\mathrm{f}}(t) - c^{\mathrm{r}}(t)||_\infty = \max_{\substack{0\le r\le n_r \\ \text{except}(0,0)}} \sum_{s=0}^{n_s} |c^{\mathrm{f}}_{r,s}(t) - c^{\mathrm{r}}_{r,s}(t)|
$$

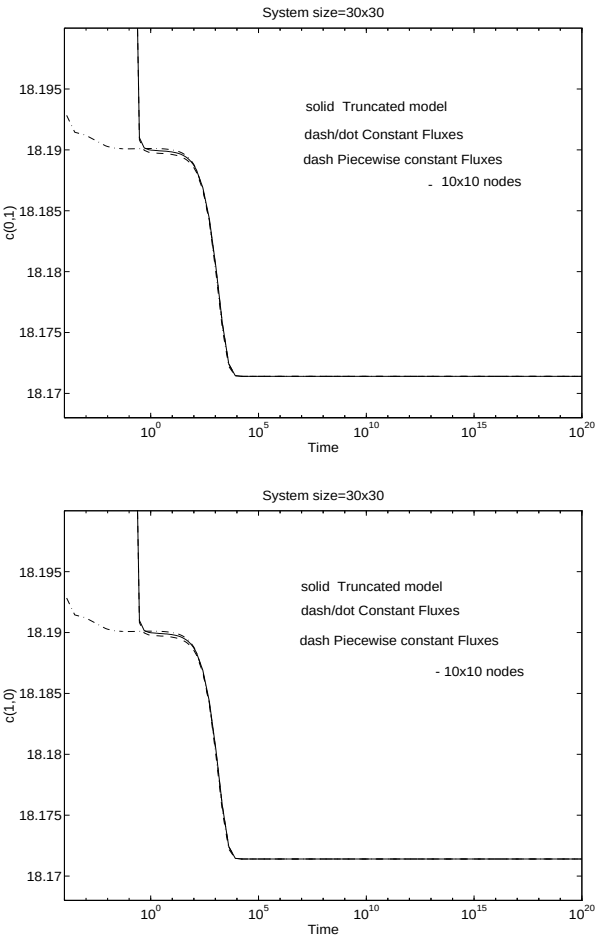

Figure 2: The monomer concentrations of the two component Becker-Döring system against time. Densities $\rho_{\mathrm{I}}(0) = \rho_{\mathrm{II}}(0) = 350$ and kinetic coefficients (11).

and

$$
||c^{\mathrm{f}}(t) - c^{\mathrm{r}}(t)||_E = \left(\sum_{(r,s)\in I_t} (c^{\mathrm{f}}_{r,s}(t) - c^{\mathrm{r}}_{r,s}(t))^2 \right)^{1/2}
$$

Figure 3 plots these errors in two different norms. For all models, the system size is 30×30, the kinetic coefficients (11 and $a = b = 10$), the initial values (13) and the densities $\rho_{\mathrm{I}} = \rho_{\mathrm{II}} = 350$. Both reduced models have excellent accuracy. The errors in both norms is less than 10^{-10} in the equilibrium phase. The accuracy of the piecewise constant models is less than 10^{-15} in the equilibrium state. We should point out that the absolute and relative local error tolerance in our *ODE* code for all models is 10^{-10}.

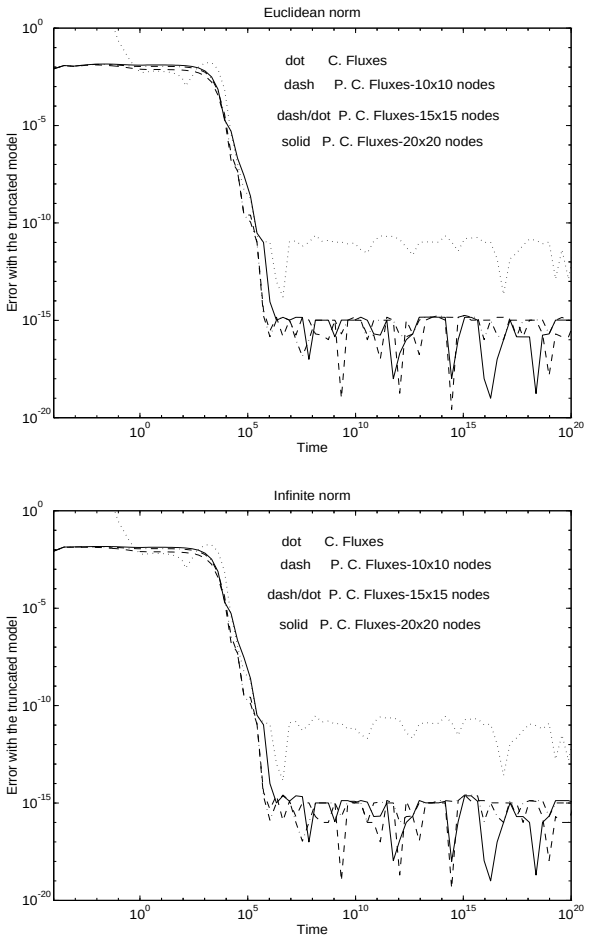

Figure 3: The errors of the constant fluxes and piecewise constant fluxes models with the truncated model in the infinite- and Euclidean-norms.

3 Discussion

The two component Becker-Döring system is formulated as in (3) and (4) and Figure 1 shows the clusters formation in this model that the cluster size can change in steps of ± 1 at each time. For numerical work, the system has to be considered as a finite dimensional model. Here we restrict the converting rates to the finite domain (5). Another way for truncating the system is, the (r, s)-cluster concentration

$$c_{r,s} = 0 \qquad \text{if } r \geq n_r \text{ or } s \geq n_s. \tag{24}$$

Finally we note that other reduced models of the one component Becker-Döring system may be extended for the two component system. Assume $c(r, s)$, converting rates $J(r, s), J'(r, s)$ and the kinetic coefficients are continuous functions of r, s, then the system can be approximated by the partial differential equation

$$\frac{\partial c}{\partial t} = \frac{\partial J}{\partial r} - \frac{\partial J'}{\partial s} \tag{25}$$

where

$$\begin{aligned} J &= -a(r,s)\, c(1,0)\, \bar{c}\, \frac{\partial}{\partial r}\left(\frac{c}{\bar{c}}\right), \\ J' &= -a'(r,s)\, c(0,1)\, \bar{c}\, \frac{\partial}{\partial s}\left(\frac{c}{\bar{c}}\right) \end{aligned}$$

and

$$\bar{c} = Q(r,s)\, c^r(1,0)\, c^s(0,1).$$

The boundary conditions for this *PDE* are very complicated and we recommend the use of the discrete form of the boundary conditions for the truncated model (7, 8), after discretizing the equation (25) by the chosen method.

References

[1] J. M. Ball, J. Carr and O. Penrose, *The Becker-Döring equations: Basic properties and asymptotic behavior of solutions,* Commun. Math. Phys. 104, 657-692(1986).

[2] R. Becker and W. Döring , *Kinetische behandlung der keimbildung in übersättigten Dämpfern,* Ann. Phy., 24-719(1935).

[3] K. E. Brenan, S. L. Campbell and L. R. Petzold, *Numerical Solution of initial-value problems in differential-algebric equations,* SIAM,Philadelphia(1996).

[4] J. Carr, D. B. Duncan and C. H. Walshaw, *Numerical approximation of a metastable system,* IMA J. Num. Anal. 15, 505-521(1995).

[5] O. Penrose, *Metastable states for the Becker-Döring cluster equations,* Commun. Math. Phys. 124, 515-541(1989).

[6] O. Penrose, J. Carr and D. G. Hall, *Kinetics of mixed micelle formation and ionic crystal nucleation,* Heriot-Watt University, Mathematics Department report(1996).

[7] L. F. Shampine, *Numerical solution of ordinay differential equation*, Chapman & Hall (1994).

[8] A. R. Soheili, *Numerical Analysis of the Coagulation-Fragmentation equations,* Ph.D. Thesis, Heriot-Watt university,Edinburgh(1997).

[9] A. R. Soheili, *Numerical Analysis of the Becker-Döring equations,* 3rd European Congress of Mathematics,Barcelona(2000).

[10] A. R. Soheili and D. B. Duncan, *Approximating the Becker-Döring cluster equations,*Applied Numerical Mathematics 37,1-29(2001).