ON AN IMPLICIT NUMERICAL METHOD
FOR THE GRINDING EQUATION

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1. Introduction

In the industry batch grinding is a frequently used unit operation. From the point of view of effectivity it is an important question how the material size changes in time. Knowing this one can determine how much time and energy is needed to get the optimal sized material. Hence one is led to study the particle size mass density function. In order to determine it we shall use one of the most wide-spread mathematical models ([1], [2], [3]). Taking this model as our basis, the solution $v(x,t) : [0, X_M] \times [0, T] \to R$ of the following integro-differential equation

(1)
$$\dot{v}(x,t) = -S(x)v(x,t) + \int_x^{X_M} S(y)b(x,y)v(y,t)dy,$$

$$v(x,0) = v_0(x) \quad \text{and} \quad x \in [0, X_M], \ t \in [0, T]$$

is the particle size mass density function of the material in the mill. Here $v_0(x) : [0, X_M] \to R_0^+$ is the particle size mass density function at $t = 0$, the selection function $S(x) : [0, X_M] \to R_0^+$ represents the fractional amount of unit mass material of size x which breaks and $b(x,y) : H \to R_0^+$ is the density function of the particles which are broken from particles of size y, and

$$H := \{(x,y) \mid 0 \le x \le y \le X_M, \ y \neq 0\},$$

X_M denotes the greatest particle size, T denotes the maximal grinding time. We can suppose that $X_M = 1$, because using a transformation of the variable we can bring it into this form.

In a previous paper [4] we have proved that under some assumptions on $S(x)$, $b(x,y)$, $v_0(x)$, equation (1) has a unique solution which is a density function. In the same paper an explicit numerical method has been given for

the approximation of the solution with error $O(h^2 + \tau)$. The method has some further properties like conservativity and nonnegativity.

In this paper we represent the solution in form of a recursive series of functions and study the smoothness of the solution. Furthermore, we present an implicit method for solving the equation numerically which has all the good properties of the explicit method, moreover it converges in second order if $v_0(x)$ is smooth. For non-smooth $v_0(x)$ we obtain first order convergence. Finally, we show that in the non-smooth case second order can be retained for an appropriately modified method.

2. The solution in function series form and its properties

Concerning the solution of (1), an existence and uniqueness theorem has been proved in [4] in the case of continuous $v_0(x)$. Now we give a more general result. We do not work out the details of the proof because it is based on the well known successive approximation method (compare [4]).

Theorem 1. *Suppose that the following conditions hold:*

(2) $S(x)$ is continuous in the interval [0,1], $v_0(x)$ is bounded and piecewise continuous in [0,1], $b(x, y)$ is continuous on H (but not necessarily on $\overline{H}$);

(3) $B := \sup\limits_{x \in [0,1]} \int\limits_x^1 |S(y)b(x, y)| dy$ is finite;

(4) $v_0(x)$, $S(x)$, $b(x, y)$ are nonnegative on their respective domains of definition;

(5) $\int\limits_0^z b(x, z) dx = 1$ for any $z \in (0, 1)$;

(6) $\int\limits_0^1 v_0(x) dx = 1$.

Then there exists a unique solution for equation (1) in the set of functions which are bounded, piecewise continuous with respect to x and continuous with respect to t.

This solution is a density function, that is nonnegative and for any $t \in [0, T]$ satisfies $\int\limits_0^1 v(x, t) dx = 1$.

Remark. The conditions (4), (5) and (6) are necessary only for the proof that the solution is a density function.

Even more can be stated about the solution.

Theorem 2. *Suppose that conditions (2) and (3) above hold. Then*

$$(7) \qquad v(x,t) = \sum_{i=0}^{\infty} \overline{v}_i(x)\frac{t^i}{i!},$$

where

$$\overline{v}_0(x) := v_0(x) \quad and$$

$$(8) \qquad \overline{v}_{i+1}(x) := -S(x)\overline{v}_i(x) + \int_x^1 S(y)b(x,y)\overline{v}_i(y)dy$$

for any $x \in [0,1]$.

Proof. Let $S_M := \max_{[0,1]} |S(x)|$ and $V_0 := \sup_{[0,1]} |v_0(x)|$. Because of (2) and (3) the recursive formula (8) is well defined for any i. Using induction we show that for $i = 0, 1, \dots, x \in [0,1]$

$$(9) \qquad \sup_{[0,1]} |\overline{v}_i(x)| \le (S_M + B)^i V_0.$$

This can be easily proved for $i = 0$, and assuming it for i, the case $i+1$ follows:

$$|\overline{v}_{i+1}(x)| \le |S(x)\overline{v}_i(x)| + \int_x^1 |S(y)b(x,y)|dy \cdot \sup_{[0,1]} |\overline{v}_i(x)| \le$$

$$\le S_M(S_M + B)^i V_0 + B(S_M + B)^i V_0 = (S_M + B)^{i+1} V_0.$$

Hence $\sum_{i=0}^{\infty} |\overline{v}_i(x)|\frac{t^i}{i!} \le V_0 e^{(S_M+B)t}$, so $\sum_{i=0}^{\infty} \overline{v}_i(x)\frac{t^i}{i!} =: v(x,t)$ exists. As the series $\sum_{i=0}^{\infty} \overline{v}_i(x)\frac{t^i}{i!}$ is absolutely and uniformly convergent and so is the series obtained by taking the derivative with respect to t, one can take the derivative and integrate it term by term with respect to x. Now using (8) we get

$$\dot{v}(x,t) = \sum_{i=0}^{\infty} \overline{v}_{i+1}(x)\frac{t^i}{i!} = \sum_{i=0}^{\infty} \left(-S(x)\overline{v}_i(x) + \int_x^1 S(y)b(x,y)\overline{v}_i(y)dy \right) \frac{t^i}{i!} =$$

$$= -S(x) \sum_{i=0}^{\infty} \overline{v}_i(x) \frac{t^i}{i!} + \int_x^1 S(y)b(x,y) \sum_{i=0}^{\infty} \overline{v}_i(y) \frac{t^i}{i!} dy =$$

$$= -S(x)v(x,t) + \int_x^1 S(y)b(x,y)v(y,t)dy.$$

Since $v(x,0) = \overline{v}_0(x) = v_0(x)$, so $\sum_{i=0}^{\infty} \overline{v}_i(x) \frac{t^i}{i!}$ satisfies indeed the equation.

Remark. From (7) and (9) it follows that $v(x,t)$ is infinitely many times differentiable with respect to t. Also from (7) and (8) it can be seen that $v(x,t)$ is as differentiable with respect to x as are $S(x)$, $b(x,y)$ and $v_0(x)$.

However, the case when $v_0(x)$ is a noncontinuous function is also important, for example when particles with size smaller than a fixed value do not exist at all, and here the function has a jump. The following theorem includes the case of noncontinuous and smooth initial function either, although in the latter one we confine ourselves only to the case $v(x,t) \in C_{2,\infty}$.

Let $I_a := (0,1] \backslash \{a\}$, where $a \in (0,1)$ and let $H_a := H \backslash \{(a,y) \mid a \leq y \leq 1\}$.

Theorem 3. *Suppose the following conditions hold:*

(10) Let $S(x)$, $b(x,y)$ be twice continuously differentiable functions on the set [0,1] and H, respectively.

(11) $v_0(x)$ is twice continuously differentiable in the points of I_a and let both one-sided limits of $v_0(x)$, $v_0'(x)$, $v_0''(x)$ at the point $x = a$ be finite.

(12) Suppose that the following suprema exist and are finite:

$$K := \sup_{(0,1]} |S(x)b(x,x)|, \qquad K' := \sup_{(0,1]} |(S(x)b(x,x))'|,$$

$$D := \sup_{(0,1]} |S(x)D_1 b(x,x)|, \qquad B := \sup_{[0,1]} \int_x^1 |S(y)b(x,y)|dy,$$

$$B' := \sup_{[0,1]} \int_x^1 |S(y)D_1 b(x,y)|dy, \qquad B'' := \sup_{[0,1]} \int_x^1 |S(y)D_1^2 b(x,y)|dy.$$

Then the unique solution for (1) is twice continuously differentiable with respect to x on the set $I_a \times [0,T]$ and both one-sided limits of $\dfrac{\partial^2 v(x,t)}{\partial x^2}$ exist at the

point x=a for any $t \in [0,T]$. If $v_0(x)$ is twice continuously differentiable on [0,1] then so is $v(x,t)$ with respect to x.

Proof. Let $S'_M := \max\limits_{[0,1]} |S'(x)|$ and $S''_M := \max\limits_{[0,1]} |S''(x)|$. By Theorem 1 the equation (1) has a unique solution which can be written in the form (7) as Theorem 2 states. Furthermore, using condition (11) the following quantity exists and is finite

$$V := \max\left(\sup_{[0,1]} |v_0(x)|, \ \sup_{I_a} |v'_0(x)|, \ \sup_{I_a} |v''_0(x)|\right).$$

For any i, $\overline{v}_i(x)$ is continuous on I_a and both one-sided limits at $x = a$ exist; this is obvious for $i = 0$ by assumptions on $v_0(x)$. For the other indices i it can be proved by induction using the recursion form (8). Since $|\overline{v}_i(x)| \leq$ $\leq (S_M + B)^i V$, the series of functions is absolutely and uniformly convergent, hence $v(x,t)$ is also continuous on I_a and it has both one-sided limits at $x = a$ and $\sup\limits_{[0,1]} |v(x,t)| \leq V \exp((S_M + B)t)$.

Using the derivative of parametric integrals we get from (8) that for any $x \in I_a$

$$\overline{v}'_0(x) = v'_0(x) \qquad \text{and}$$
(13)
$$\overline{v}'_{i+1}(x) = -S(x)\overline{v}'_i(x) - S'(x)\overline{v}_i(x) - S(x)b(x,x)\overline{v}_i +$$
$$+ \int_x^1 S(y)D_1 b(x,y)\overline{v}_i(y)dy.$$

Now again by induction one can see that for any i the derivative $\overline{v}'_i(x)$ is continuous on I_a and its both one-sided limits exist. It is easy to prove that for any $x \in I_a$
$$|\overline{v}'_i(x)| \leq (S_M + S'_M + K + B + B')^i V,$$

consequently $\sum\limits_{i=0}^{\infty} \overline{v}'_i(x)\dfrac{t^i}{i!}$ converges absolutely and uniformly in I_a, therefore

$\dfrac{\partial v(x,t)}{\partial x}$ is also continuous, it has both one-sided limits at $x = a$ and
$$\sup_{I_a} \left|\frac{\partial v(x,t)}{\partial x}\right| \leq V \exp((S_M + S'_M + K + B + B')t).$$

This last statement can be proved for $\dfrac{\partial^2 v(x,t)}{\partial x^2}$ in a similar manner. Now for $x \in I_a$

$$\overline{v}_0''(x) = v_0''(x),$$

$$\overline{v}_{i+1}'' = -S(x)\overline{v}_i''(x) - 2S'(x)\overline{v}_i'(x) - S''(x)\overline{v}_i(x) -$$

(14)

$$- S(x)b(x,x)\overline{v}_i'(x) - (S(x)b(x,x))'\overline{v}_i(x) -$$

$$- S(x)D_1 b(x,x)\overline{v}_i(x) + \int\limits_x^1 S(y)D_1^2 b(x,y)\overline{v}_i(y)dy.$$

Once again using induction one can see that $\overline{v}_i''(x)$ is continuous on I_a and has both one-sided limits at $x = a$, and for any $x \in I_a$

$$|\overline{v}_i''(x)| \le (S_M + 2S_M' + S_M'' + K + K' + D + B + B' + B'')^i V.$$

From this inequality it follows that $\displaystyle\sum_{i=0}^{\infty} \overline{v}_i''(x)\dfrac{t^i}{i!}$ converges absolutely and uniformly on I_a, therefore $\dfrac{\partial^2 v(x,t)}{\partial x^2}$ is continuous on I_a and has both one-sided limits at $x = a$ and

$$\sup_{I_a} \left|\dfrac{\partial^2 v(x,t)}{\partial x^2}\right| \le V \exp((S_M + 2S_M' + S_M'' + K + K' + D + B + B' + B'')t).$$

It can be easily seen that if $v_0(x)$ is twice continuously differentiable on $[0,1]$, with some modification of the above idea we get that $v(x,t)$ is also twice continuously differentiable with respect to x.

Remarks. 1) One can read it from Theorem 3 that $v(x,t)$, $\dfrac{\partial v(x,t)}{\partial x}$, $\dfrac{\partial^2 v(x,t)}{\partial x^2}$ are uniformly bounded on the set $I_a \times [0,T]$.

2) It can be easily seen that if the jump of $v_0(x)$ at $x = a$ is u then $v(x,t)$ has a jump of size $e^{-S(a)t}u$ tending to 0 as $t \to \infty$.

We mention that assuming $S(x) > 0$, $b(x,y) > 0$ if $x > 0$, it can be proved that not only the value of the jump tends to zero but $v(x,t)$ as well [5].

In the literature ([6], [7]) the following special cases are widely used:

(15)
$$S(x) = kx^q \quad \text{and} \quad b(x,y) = \dfrac{x^{p-1}}{y^p}$$

where $q \geq 0$, $k > 0$ and $p > 0$ are given constants.

Corollary. *If condition (11) holds for $v_0(x)$ and the above parameters p and q satisfy either of the following conditions*

$$p = q = 1;$$
$$p = 1, \qquad q \geq 2;$$
(16) $\qquad\qquad p = 2, \qquad q \geq 2;$
$$p = 3, \qquad q > 2;$$
$$p > 3, \qquad q \geq 2,$$

then the unique solution for the equation (1) is twice continuously differentiable on $I_a \times [0, T]$ and $\dfrac{\partial^2 v(x, t)}{\partial x^2}$ has both one-sided limits at $x = a$ for any $t \in [0, T]$. If $v_0(x)$ is twice continuously differentiable on [0,1] then so is $v(x, t)$.

Proof. The conditions of Theorem 3 hold. It is enough to check whether (12) holds. Instead of a detailed proof we restrict ourselves to the following list (which exhausts all cases of (16)):

- K is finite if $q \geq 1$;
- K' is finite if $q \geq 2$ or if $q = 1$;
- D is finite if $q \geq 2$ or if $p = 1$;
- B is finite if $q > 0$, $p \geq 1$ or if $q = 0$, $p > 1$;
- B' is finite if $p = 1$ or if $q > 1$, $p \geq 2$ or if $q = 1$, $p > 2$;
- B'' is finite if $p = 1$ or if $p = 2$ or if $q > 2$, $p \geq 3$ or if $q = 2$, $p > 3$.

3. The implicit method and its general properties

The exact solution to (1) is known only in some special cases ([7], [8]). Therefore it is important to know how (1) can be solved numerically. However we want to approximate a density function, hence above the convergence and nonnegativity we require the approximate solution to satisfy a discrete conservation law in accordance with the equality $\int_0^1 v(x, t) dx = 1$. In this manner we get the discrete model of our process.

As it has been already mentioned, in [4] an explicit method was proposed which satisfies the above requirement, but has only a first order convergence in τ. In this point we describe a more efficient implicit version of the method.

Let us introduce the following notations:

Let N, M be natural numbers, $\tau := \dfrac{T}{M}$, $h := \dfrac{1}{N}$, $t_m := m \cdot \tau$, $x_i := ih$, $S_i :=$
$:= S(x_i)$, $b_{ij} := b(x_i, x_j)$ and $v_{im} := v(x_i, t_m)$, where $m = 0, 1, \ldots, M$ and
$i, j = 0, 1, \ldots, N$.

We approximate the derivative with respect to t by a difference quotient
and the integral by the trapezoidal rule. We define the "discrete" conservation
law to hold if $\sum\limits_{i=0}^{N} y_{im} \gamma_i h = 1$ (where $\gamma_0 = \gamma_N = 1/2$ and $\gamma_1 = \gamma_2 = \ldots =$
$= \gamma_{N-1} = 1$) for the numerical solution $\{y_{im}\}$.

To achieve this we modify the trapezoidal rule choosing the following
recursive implicit system of equations for the approximation of (1):

(17)

$$y_{i0} = \frac{v_0(x_i)}{\sum\limits_{i=0}^{N} v_0(x_i)\gamma_i h} \qquad i = 0, 1, \ldots, N,$$

$$y_{0m+1} = y_{0m} + \frac{\tau}{2} \sum_{j=1}^{N} S_j \, \tilde{b}_{0j} \, \omega_{0j} h(y_{jm+1} + y_{jm}),$$

$$y_{im+1} = y_{im} - \frac{\tau}{2} S_i (y_{im+1} + y_{im}) + \frac{\tau}{2} \sum_{j=1}^{N} S_j \, \tilde{b}_{ij} \, \omega_{ij} h(y_{jm+1} + y_{jm}),$$

$$i = 1, \ldots, N - 1,$$

$$y_{Nm+1} = y_{Nm} - \frac{\tau}{2} S_N (y_{Nm+1} + y_{Nm}),$$

where

$$\omega_{ij} = \begin{cases} 1/2, & \text{if } i = j \text{ or if } j = N, \\[2mm] 1, & \text{if } i < j \quad (i = 0, 1, \ldots, N-1; \; j = 1, 2, \ldots, N), \end{cases}$$

$$\tilde{\omega}_{ij} = \begin{cases} 1/2, & \text{if } i = j \text{ or if } i = 0, \\[2mm] 1, & \text{if } i < j \; (i = 0, 1, \ldots, j; \; j = 1, 2, \ldots, N) \end{cases}$$

and

$$\tilde{b}_{ij} = \begin{cases} \dfrac{b_{ij}}{\sum\limits_{k=0}^{j} b_{kj}\tilde{\omega}_{kj} h}, & \text{if } j = 0, 1, \ldots, N-1; \, i = 0, 1, \ldots, j \text{ and } i^2 + j^2 \neq 0, \\[4mm] \dfrac{b_{iN}}{\sum\limits_{k=0}^{N-1} b_{kN}\tilde{\omega}_{kN} h}, & \text{if } j = N, \, i = 0, 1, \ldots, N. \end{cases}$$

We can rewrite the recursion in the form

(18)
$$\underline{y}_0 = \frac{1}{\sum_{i=0}^{N} v_0(x_i)\gamma_i h} \cdot \underline{v}_0,$$

$$\underline{y}_{m+1} = \underline{y}_m + \frac{1}{2}(D - I)(\underline{y}_{m+1} + \underline{y}_m) \qquad (m = 0, 1, \ldots, M-1),$$

where $D = (d_{ij})_{(N+1)\times(N+1)}$ and

(19)
$$d_{ij} = \begin{cases} 1 - \tau S_i + \tau S_i \, \tilde{b}_{ii} \, \omega_{ii} h, & \text{if } i = j \text{ and } i \neq 0, N; \\[2mm] 1, & \text{if } i = j = 0; \\[2mm] \tau S_j \, \tilde{b}_{ij} \, \omega_{ij} h, & \text{if } i < j; \\[2mm] 1 - \tau S_N, & \text{if } i = j = N; \\[2mm] 0, & \text{if } i > j. \end{cases}$$

We are going to prove that the values y_{im} are nonnegative and satisfy the discrete conservation law.

Theorem 4. *Assume that condition (4) holds. Then y_{im} defined by (17) satisfy the equality $\sum_{i=0}^{N} y_{im}\gamma_i h = 1$, moreover, if $\tau \leq \dfrac{1}{S_M}$, then $y_{im} \geq 0$.*

Proof. The statement is obvious for $m = 0$. Now we assume that $\sum_{i=0}^{N} y_{ik}\gamma_i h = 1$ for $k = 0, 1, \ldots, m$. Let us prove it for $k = m + 1$. We have from (17)

$$\sum_{i=0}^{N} y_{im+1}\gamma_i h = \sum_{i=0}^{N} y_{im}\gamma_i h - \frac{\tau}{2}\sum_{i=1}^{N} S_i(y_{im+1} + y_{im})\gamma_i h + \Sigma_N,$$

where

$$\Sigma_N := \frac{\tau}{2}\gamma_0 h \sum_{j=1}^{N} S_j (y_{jm+1} + y_{jm}) \, \widetilde{b}_{0j} \, \omega_{0j} h +$$

$$+ \frac{\tau}{2} \sum_{i=1}^{N-1} \gamma_i h \sum_{j=i}^{N} S_j (y_{jm+1} + y_{jm}) \, \widetilde{b}_{ij} \, \omega_{ij} h =$$

$$= \frac{\tau}{2}\gamma_0 h \sum_{j=1}^{N} S_j (y_{jm+1} + y_{jm}) \, \widetilde{b}_{0j} \, \omega_{0j} h +$$

$$+ \frac{\tau}{2} \sum_{j=1}^{N-1} \sum_{i=1}^{j} \gamma_i h S_j (y_{jm+1} + y_{jm}) \, \widetilde{b}_{ij} \, \omega_{ij} h +$$

$$+ \frac{\tau}{2} \sum_{i=1}^{N-1} \gamma_i h S_N (y_{Nm+1} + y_{Nm}) \, \widetilde{b}_{iN} \, \omega_{iN} h =$$

$$= \frac{\tau}{2} \sum_{j=1}^{N-1} \sum_{i=0}^{j} \gamma_i h S_j (y_{jm+1} + y_{jm}) \, \widetilde{b}_{ij} \, \omega_{ij} h +$$

$$+ \frac{\tau}{2} \sum_{i=0}^{N-1} \gamma_i h S_N (y_{Nm+1} + y_{Nm}) \, \widetilde{b}_{iN} \, \omega_{iN} h.$$

Therefore the following equality holds:

$$\sum_{i=0}^{N} y_{im+1}\gamma_i h =$$

$$= \sum_{i=0}^{N} y_{im}\gamma_i h - \frac{\tau}{2} \sum_{j=1}^{N-1} (y_{jm+1} + y_{jm}) S_j h \left(\gamma_j - \sum_{i=0}^{j} \gamma_i \, \widetilde{b}_{ij} \, \omega_{ij} h \right) -$$

$$- \frac{\tau}{2} (y_{Nm+1} + y_{Nm}) S_N h \left(\gamma_N - \sum_{i=0}^{N-1} \gamma_i \, \widetilde{b}_{iN} \, \omega_{iN} h \right).$$

It can be easily seen that in the case $j = 1, \ldots, N-1$ and $i = 0, \ldots, N-1$, we have $\gamma_i \omega_{ij} = \widetilde{\omega}_{ij}$, furthermore if $i = 0, \ldots, N-1$ then $\gamma_i \omega_{iN} = \frac{1}{2} \widetilde{\omega}_{iN}$. Hence for $j = 1, \ldots, N-1$ there holds

$$\sum_{i=0}^{j} \gamma_i \, \widetilde{b}_{ij} \, \omega_{ij} h = \sum_{i=0}^{j} \gamma_i \frac{b_{ij}\omega_{ij} h}{\sum\limits_{i=0}^{j} b_{kj} \, \widetilde{\omega}_{kj} \, h} = 1 = \gamma_j \qquad \text{and}$$

$$\sum_{i=0}^{N-1} \gamma_i \, \widetilde{b}_{iN} \, \omega_{iN} h = \sum_{i=0}^{N-1} \gamma_i \frac{b_{iN} \omega_{iN} h}{\sum\limits_{i=0}^{N-1} b_{kN} \, \widetilde{\omega}_{kN} \, h} = \frac{1}{2} = \gamma_N.$$

This calls forth the equality $\sum\limits_{i=0}^{N} y_{im+1} \gamma_i h = \sum\limits_{i=0}^{N} y_{im} \gamma_i h = 1$ and proves the first part of the statement.

One can see from (19) that if τ is sufficiently small then the matrix $I - \frac{1}{3}D$ is invertible, so we get from (18) that

(20) $\underline{y}_{m+1} = \widetilde{D} \, \underline{y}_m$,   where $\widetilde{D} := \frac{1}{3}\left(I - \frac{1}{3}D\right)^{-1}(D + I).$

If $\tau \le 1/S_M$, D is nonnegative. Then using

$$\left(I - \frac{1}{3}D\right)^{-1} = I + \frac{D}{3} + \left(\frac{D}{3}\right)^2 + \cdots,$$

the nonnegativity of $\underline{y}_{m+1}$ follows from the nonnegativity of $\underline{y}_m$. Since $\underline{y}_0 \ge 0$, the second part of the statement is also proved.

Remark. The method given by the recursion (17) is almost explicit, because $y_{Nm+1}, \ldots, y_{0m+1}$ can be expressed by backsubstitution. Hence the method requires $O(mN^2)$ steps for computing the vector $\underline{y}_{m+1}$ which is about the same as in the case of the explicit method.

4. Convergence and stability

In this part we examine the convergence and stability of above method. We need some assumptions.

(21) $\dfrac{\partial^2 (S(y)b(x,y))}{\partial y^2}$ exists for any $(x, y) \in H$, and

$$W := \sup_{H} \left| \frac{\partial^2 (S(y)b(x,y))}{\partial y^2} \right| \quad \text{is finite.}$$

(22) $\dfrac{\partial^2 b(x,y)}{\partial x^2}$ exists for any $(x, y) \in H$, and

$$B_x := \sup_{H} |S(y)b(x,y)B(y)| \quad \text{is finite, where}$$

$$B(y) := \sup_{x \in [0,y]} \left| \frac{\partial^2 b(x,y)}{\partial y^2} \right|.$$

(23)   Let $\lim_{(x,y) \to (0,0)} S(y)b(x,y) = 0$.

(24)   Let $\min_{j=1,\ldots,N-1} \sum_{k=0}^{j} b_{kj} \, \tilde{\omega}_{kj} \, h \geq \frac{1}{2}$ and $\sum_{k=0}^{N-1} b_{kN} \, \tilde{\omega}_{kN} \, h \geq \frac{1}{2}$

(this condition is not very restrictive since the approximate sum of the integral $\int_0^{x_j} b(x, x_j)dx = 1$; this means that h has to be chosen sufficiently small).

(25)   Let $S(0) = 0$

(this is natural assumption, because particles with size 0 cannot break).

Now we prove the following

Theorem 5. *Assume (3)-(6), (10), (12), (21)-(25) and let $v_0(x)$ be twice continuously differentiable on $[0,1]$. In the case $V_2 := \max_{[0,1]} \left| \frac{d^2 v_0(x)}{dx^2} \right| > 0$ let $h < \left(\frac{6}{V_2} \right)^{1/2}$ and in the case $V_2 = 0$ let h be arbitrary. Finally, assume $\tau \leq \frac{1}{S_M}$. Then there holds the error estimation*

$$|v(x_i, t_m) - y_{im}| \leq c_6 h^2 + c_7 \tau^2 \qquad (m = 0, 1, \ldots, M; \quad i = 0, 1, \ldots, N)$$

where the approximate values y_{im} are defined by the recursion (17), and c_6, c_7 are constants independent of N and M.

Proof. By Theorem 2 $v(x,t)$ is three times continuously differentiable with respect to t. Let $V_T := \max_{[0,1] \times [0,T]} \left| \frac{\partial^3 v(x,t)}{\partial t^3} \right|$. Using the Taylor series expansion the following inequalities are found to hold:

(26)
$$\left\| \frac{\dot{v}_{m+1} + \dot{v}_m}{2} - \dot{v}_{m+1/2} \right\|_{\infty} \leq V_T \frac{\tau^2}{8} \qquad \text{and}$$

$$\left\| \frac{v_{m+1} - v_m}{\tau} - \dot{v}_{m+1/2} \right\|_{\infty} \leq V_T \frac{\tau^2}{24},$$

where

$$\underline{v}_{m+1/2} = \left(v\left(x_0, t_m + \frac{\tau}{2}\right), v\left(x_1, t_m + \frac{\tau}{2}\right), \ldots, v\left(x_N, t_m + \frac{\tau}{2}\right) \right)^T \quad \text{and}$$

$$\underline{\dot v}_{m+1/2} = \left(\frac{\partial v}{\partial t}\left(x_0, t_m + \frac{\tau}{2}\right), \frac{\partial v}{\partial t}\left(x_1, t_m + \frac{\tau}{2}\right), \ldots, \frac{\partial v}{\partial t}\left(x_N, t_m + \frac{\tau}{2}\right) \right)^T$$

and the other expressions are obtained similarly.

By Theorem 3 $v(x, t)$ is twice continuously differentiable with respect to x, too, hence $V := \max_{[0,1] \times [0,T]} |v(x,t)|$ is finite, and because of (10) $S(y)b(x, y)v(y, t)$ is twice continuously differentiable with respect to y on the set $H \times [0, T]$. The condition (21) assures that $R := \sup_{H \times [0,T]} \left| \dfrac{\partial^2 (S(y)b(x, y)v(y, t))}{\partial y^2} \right|$ is finite.

Therefore

$$(27) \qquad \left| \int_{x_0}^{1} S(y)b(x_0, y)v(y, t_m)dy - \sum_{j=1}^{N} S_j b_{0j} v_{jm} \omega_{0j} h \right| \leq \frac{R}{12} h^2,$$

where we have used that the term corresponding to $j = 0$ is zero because of (23).

Further for $i = 1, \ldots, N - 1$ we have

$$(28) \qquad \left| \int_{x_i}^{1} S(y)b(x_i, y)v(y, t_m)dy - \sum_{j=i}^{N} S_j b_{ij} v_{jm} \omega_{ij} h \right| \leq \frac{R}{12} h^2.$$

Moreover

$$\left| \int_{x_0}^{x_\ell} b(x, x_\ell)dx - \sum_{k=0}^{\ell} b_{k\ell} \tilde\omega_{k\ell} h \right| \leq \frac{B(x_\ell)}{12} h^2 \quad \text{for} \quad \ell = 1, \ldots, N,$$

hence for $j = 1, \ldots, N - 1$ and $i = 0, \ldots, j$ it follows that

$$S_j \tilde b_{ij} =$$

$$= S_j b_{ij} \frac{1}{\displaystyle\sum_{k=0}^{j} b_{kj} \tilde\omega_{kN} h} \leq S_j b_{ij} \left(1 + \frac{B(x_j)}{\displaystyle\sum_{k=0}^{j} b_{kj} \tilde\omega_{kj} h} \frac{h^2}{12} \right) \leq S_j b_{ij} + c_1 h^2$$

and for $i = 0, 1, \ldots, N$

$$S_N \, \tilde{b}_{iN} \le S_N b_{iN} \left(1 + \frac{B(x_N)}{\sum\limits_{k=0}^{N-1} b_{kN} \, \tilde{\omega}_{kN} \, h} \frac{h^2}{12} + \frac{\frac{1}{2} b_{NN} h}{\sum\limits_{k=0}^{N-1} b_{kN} \, \tilde{\omega}_{kN} \, h} \right) \le S_N b_{iN} + c_2 h$$

with appropriate constants c_1 and c_2 which are independent of N, M.

The last two inequalities require (22) and (24). So

$$(29) \qquad \begin{aligned} \sum_{j=1}^{N} S_j \, \tilde{b}_{0j} \, v_{jm} \omega_{0j} h &\le \sum_{j=1}^{N} S_j b_{0j} v_{jm} \omega_{0j} h + (c_1 + c_2) V h^2 = \\ &= \sum_{j=1}^{N} S_j b_{0j} v_{jm} \omega_{0j} h + c_3 h^2 \end{aligned}$$

and for $i = 1, \ldots, N-1$

$$(30) \qquad \begin{aligned} \sum_{j=i}^{N} S_j \, \tilde{b}_{ij} \, v_{jm} \omega_{ij} h &\le \sum_{j=i}^{N} S_j b_{ij} v_{jm} \omega_{ij} h + (c_1 + c_2) V h^2 = \\ &= \sum_{j=i}^{N} S_j b_{ij} v_{jm} \omega_{ij} h + c_3 h^2. \end{aligned}$$

Using the inequalities (26)-(29) and the assumption (25) we get

$$(31) \qquad \underline{v}_{m+1} = \underline{v}_m + \frac{1}{2}(D - I)(\underline{v}_{m+1} + \underline{v}_m) + O(\tau(\tau^2 + h^2)).$$

Let $\underline{z}_m = \underline{v}_m - \underline{y}_m$. Then by (30)

$$\|\underline{z}_{m+1}\|_\infty \le \| \tilde{D} \|_\infty \|\underline{z}_m\|_\infty + \frac{2}{3} \left\| \left(I - \frac{1}{3} D \right)^{-1} \right\|_\infty \left(\left(\frac{R}{12} + c_3 \right) h^2 + \frac{V_T}{6} \tau^2 \right) \tau.$$

Therefore

$$(32) \qquad \|\underline{z}_{m+1}\|_\infty \le \| \tilde{D} \|_\infty^{m+1} \|\underline{z}_0\|_\infty +$$

$$+ \left[\frac{2}{3} \sum_{i=0}^{m} \| \tilde{D} \|_\infty^{i} \left\| \left(I - \frac{1}{3} D \right)^{-1} \right\|_\infty \left(\left(\frac{R}{12} + c_3 \right) h^2 + \frac{V_T}{6} \tau^2 \right) \tau \right].$$

We now estimate $\| \tilde{D} \|_\infty$

$$(33) \quad \| \tilde{D} \|_\infty \le \frac{1}{3} \left\| \left(I - \frac{1}{3}D \right)^{-1} \right\|_\infty \| D + I \|_\infty \le \frac{1}{3 - \|D\|_\infty}(1 + \|D\|_\infty).$$

If $\tau \le \dfrac{1}{S_M}$, the elements of D are nonnegative, hence we can estimate the row-sums as follows

$$D_0 := 1 + \tau \sum_{j=1}^N S_j \, \tilde{b}_{0j} \, \omega_{0j} h \le 1 + \tau \sum_{j=1}^N S_j b_{0j} \omega_{0j} h + \tau(c_1 + c_2)h^2 \le$$

$$\le 1 + \tau \left(B + \frac{Wh^2}{12} \right) + \tau(c_1 + c_2)h^2 \le 1 + c_4 \tau,$$

$$D_i := 1 - \tau S_i + \tau \sum_{j=i}^N S_j \, \tilde{b}_{ij} \, \omega_{ij} h \le 1 + \tau \sum_{j=i}^N S_j b_{ij} \omega_{ij} h + \tau(c_1 + c_2)h^2 \le$$

$$\le 1 + \tau \left(B + \frac{Wh^2}{12} \right) + \tau(c_1 + c_2)h^2 \le 1 + c_4 \tau \quad (i = 1, \ldots, N-1)$$

and

$$D_N := 1 - \tau S_N \le 1 + c_4 \tau.$$

Deriving these inequalities we have used the assumption (21). Therefore $\|D\|_\infty \le 1 + c_4\tau$, hence by (33)

$$(34) \quad \| \tilde{D} \|_\infty \le 1 + \overline{c_4}\tau \quad \text{where} \quad \overline{c_4} := \frac{2c_4}{2 - c_4 \tau}.$$

Finally,

$$(35) \quad \|\underline{z}_0\|_\infty = \left\| \underline{v}_0 - \frac{1}{\sum_{i=0}^N v_0 \gamma_i h} v_0 \right\|_\infty \le \|\underline{v}_0\|_\infty \frac{\frac{V_2 h^2}{12}}{1 - \frac{V_2 h^2}{12}} \le c_5 h^2$$

with an appropriate constant c_5. By (34), (35) and (32) there holds

$$\|\underline{z}_{m+1}\|_\infty \le$$

$$\leq (1 + \bar{c}_4 \tau)^{m+1} c_5 h^2 + \sum_{i=0}^{m} (1 + \bar{c}_4 \tau)^i \frac{2}{2 - c_4 \tau} \left(\left(\frac{R}{12} + c_3 \right) h^2 + \frac{V_T}{6} \tau^2 \right) \tau \leq$$

$$\leq e^{\bar{c}_4 T} \left\{ \left[c_5 + \frac{2}{2 - c_4 \tau} \left(\frac{TR}{12} + Tc_3 \right) \right] h^2 + \frac{2T}{2 - c_4 \tau} \cdot \frac{V_T}{6} \tau^2 \right\} = c_6 h^2 + c_7 \tau^2.$$

Now comparing (20) and (34) one can see that the method is stable.

5. The case of noncontinuous initial function

As mentioned in the point 2, in practice there is also important the case when $v_0(x)$ has a jump at $x = a$. The method (17) will converge under certain conditions also in this case, but the order of convergence decreases. More precisely, if the conditions (3)-(6), (10)-(12) and (21)-(25) hold, furthermore h and τ are sufficiently small, then the error of approximation of the solution is $O(h + \tau^2)$.

However, we now give a new method which converges in second order also in the case of a piecewise continuous initial function, but the jump point has to coincide with a mesh point. For the sake of simplicity we consider the case of a uniform mesh only.

We assume that $v(x, t)$ has both one-sided limits at $x = a$ for any t. Let these limits be denoted by $v_0(x_k-)$ and $v_0(x_k+)$ in case of the initial function and by $v(x_k-, t_m)$ and $v(x_k+, t_m)$ in the general case. The assumptions of Theorem 3 assure the existence of these limits. The method (which essentially is a trapezoidal rule with two v-values at $x_k = a$) can now be described as follows:

$$\hat{\underline{y}}_0 = \frac{1}{\sum\limits_{\substack{i=0 \\ i \neq k}}^{N} v_0(x_i) \gamma_i h + \frac{h}{2} (v_0(x_k-) + v_0(x_k+))} \hat{\underline{v}}_0,$$

(40)

$$\hat{\underline{y}}_{m+1} = \hat{\underline{y}}_m + \frac{1}{2} (\hat{D} - I)(\hat{\underline{y}}_{m+1} + \hat{\underline{y}}_m) \qquad (m = 0, 1, \dots, M - 1),$$

where $\hat{D} = (\hat{d}_{ij})_{(N+2)\times(N+2)}$,

(41)

$$
\hat{d}_{ij} = \begin{cases}
1, & \text{if } i = j = 0, \\
1 - \tau S_i + \tau S_i \, \tilde{b}_{ii} \, \omega_{ii} h, & \text{if } i = j; \ i = 1, \ldots, k-1, \\
1 - \tau S_k, & \text{if } i = j = k, \\
1 - \tau S_k + \tau S_k \, \tilde{b}_{kk} \, \dfrac{h}{2}, & \text{if } i = j = k+1, \\
1 - \tau S_{i-1} + \tau S_{i-1} \, \tilde{b}_{i-1,i-1} \, \omega_{i-1,i-1} h, & \text{if } i = j; \ i = k+2, \ldots, N, \\
1 - \tau S_N, & \text{if } i = j = N+1, \\
\tau S_j \, \tilde{b}_{ij} \, \omega_{ij} h, & \text{if } i = 0, \ldots, j-1; \\
 & \quad j = 1, \ldots, k-1, \\
\tau S_k \, \tilde{b}_{ik} \, \dfrac{h}{2}, & \text{if } i = 0, \ldots, j-1; \\
 & \quad j = k, k+1, \\
\tau S_{j-1} \, \tilde{b}_{i,j-1} \, \omega_{i,j-1} h, & \text{if } i = 0, \ldots, k; \\
 & \quad j = k+2, \ldots, N+1, \\
\tau S_{j-1} \, \tilde{b}_{i-1,j-1} \, \omega_{i-1,j-1} h, & \text{if } i = k+1, \ldots, j-1; \\
 & \quad j = k+2, \ldots, N+1, \\
0, & \text{if } i = j+1, \ldots, N+1; \\
 & \quad j = 0, \ldots, N,
\end{cases}
$$

where

$$
\hat{\underline{y}}_m = (\hat{y}_{0m}, \hat{y}_{1m}, \ldots, \hat{y}_{k-1,m}, \hat{y}_{km}^{-}, \hat{y}_{km}^{+}, \hat{y}_{k+1,m}, \ldots, \hat{y}_{Nm})^T
$$

and

$$
\hat{\underline{v}}_0 = (v_0(x_0), v_0(x_1), \ldots, v_0(x_{k-1}), v_0(x_k-), v_0(x_k+), v_0(x_{k+1}), \ldots, v_0(x_N))^T.
$$

If τ is sufficiently small then $I - \dfrac{1}{3}\hat{D}$ is invertible, hence from (40) we get

(42)
$$
\hat{\underline{y}}_{m+1} = \overline{D}\hat{\underline{y}}_m,
$$

where

$$
\overline{D} := \frac{1}{3}\left(I - \frac{1}{3}\hat{D}\right)^{-1}(\hat{D} + I).
$$

Similarly as in the case of recursion (17) one can prove that $\hat{\underline{y}}_m$ is nonnegative if condition (4) holds. The details of proof are not worked out here, they are similar to the case (17). We formulate now

Theorem 6. *Suppose that the assumptions (3)-(6), (10)-(12) and (21)-(25) hold. Let $h \leq \left(\dfrac{6}{V_0}\right)^{1/2}$ if $V_a := \sup\limits_{I_a} \left|\dfrac{d^2 v_0(x)}{dx^2}\right| > 0$ and h be arbitrary if*

$V_a = 0$ and, finally, assume that $\tau \le \dfrac{1}{S_M}$. Then the following error estimation is true:

$$|v(x_i, t_m) - \hat{y}_{im}| \le c_{10}h^2 + c_7\tau^2$$

$$(m = 0, 1, \ldots, M;\ i = 0, 1, \ldots, k-1, k+1, \ldots, N)$$

and

$$|v(x_k-, t_m) - \hat{y}_{km}^-| \le c_{10}h^2 + c_7\tau^2,$$

$$|v(x_k+, t_m) - \hat{y}_{km}^+| \le c_{10}h^2 + c_7\tau^2,$$

where c_{10}, c_7 are constants independent of N and M.

Proof. The proof is the same as that of Theorem 5 with some modifications. The differences are in the proof of inequalities (27), (28) and (33). On one hand, because of Theorem 3 and assumptions (10) and (21),

$$R_a := \sup_{H_a \times [0,T]} \left| \frac{\partial^2(S(y)b(x, y)v(y, t))}{\partial y^2} \right|$$

exists and is finite. Hence for $x_0 < x_k = a < x_{k+1}$,

$$\left| \int_{x_0}^{1} S(y)b(x_0, y)v(y, t_m)dy - \sum_{\substack{j=1 \\ j \ne k}}^{N} S_j b_{0j} v_{jm}\omega_{0j}h - \frac{h}{2}S_k b_{0k}(v_{km}^- + v_{km}^+) \right| \le$$

(43)
$$\le \left| \int_{x_0}^{x_k} S(y)b(x_0, y)v(y, t_m)dy - \sum_{j=1}^{k-1} S_j b_{0j} v_{jm}\omega_{0j}h - \frac{h}{2}S_k b_{0k}v_{km}^- \right| +$$

$$+ \left| \int_{x_k}^{1} S(y)b(x_0, y)v(y, t_m)dy - \sum_{j=k+1}^{N} S_j b_{0j} v_{jm}\omega_{0j}h - \frac{h}{2}S_k b_{0k}v_{km}^+ \right| \le$$

$$\le \frac{x_k}{12}R_a h^2 + \frac{1 - x_k}{12}R_a h^2 = \frac{R_a h^2}{12}.$$

Similarly one can show for $i = 1, \ldots, N-1$ also that the difference between the integral $\displaystyle\int_{x_i}^{1} S(y)b(x_i, y)v(y, t_m)dy$ and its approximate sum (which uses the left-side and right-side limits) is less than or equal to $\dfrac{R_a h^2}{12}$.

The right-hand side of (32) changes, of course. Instead of (32) we obtain

$$\|\hat{z}_{m+1}\|_\infty \le$$

$$\le \|\overline{D}\|_\infty^{m+1}\|\hat{z}_0\|_\infty + \frac{2}{3}\sum_{i=0}^{m}\|\overline{D}\|_\infty^i \left\|\left(I - \frac{1}{3}\hat{D}\right)^{-1}\right\|_\infty \left(\left(\frac{R_a}{12} + c_3\right)h^2 + \frac{V_T}{6}\tau^2\right)\tau.$$

We get

$$\|\hat{z}_0\|_\infty \le \|\hat{v}_0\|_\infty \left|\frac{1 - \left[\sum_{\substack{i=0\\i\neq k}}^{N} v_0(x_i)\gamma_i h + \frac{h}{2}(v_0(x_k-) + v_0(x_k+))\right]}{\sum_{\substack{i=0\\i\neq k}}^{N} v_0(x_i)\gamma_i h + \frac{h}{2}(v_0(x_k-) + v_0(x_k+))}\right| \le c_8 h^2,$$

because using $1 = \int_0^1 v_o(x)dx$ one can prove that

$$\left|1 - \left[\sum_{\substack{i=0\\i\neq k}}^{N} v_0(x_i)\gamma_i h + \frac{h}{2}(v_0(x_k-) + v_0(x_k+))\right]\right| \le c_9 h^2$$

with a constant c_9 (see the derivation of inequality (43)).

Finally, an estimation similar to (34) can be written for $\|\overline{D}\|_\infty$ since

(44) $$\|\overline{D}\|_\infty = \|\tilde{D}\|_\infty.$$

Therefore

$$\|\hat{z}_{m+1}\|_\infty \le e^{\bar{c}_4 T}\left\{\left[c_8 + \left(\frac{TR_a}{12} + Tc_9\right)\cdot\frac{2}{2 - c_4\tau}\right]h^2 + \frac{2T}{2 - c_4\tau}\cdot\frac{V_T}{6}\tau^2\right\} =$$

$$= c_{10}h^2 + c_7\tau^2.$$

Remark. The method (40) is also stable as it can be seen from (44) and (42).

6. Numerical results

We illustrate the accuracy of the method by some examples corresponding to (15). The case $p = q$ is examined because in that case the exact solution is known, namely

$$v(x,t) = e^{-kx^p t}(v_0(x)kpx^{p-1}tR_0(x)), \quad \text{where} \quad R_0(x) := \int\limits_x^1 v_0(z)dz.$$

The results of computations support the given estimations.

Table 1 contains the deviation of computed and exact solution values in the discrete maximum norm for some values $p(= q)$ if the initial function is smooth. Since the order of convergence proved theoretically is $c_6 h^2 + c_7 \tau^2$, we have chosen $\tau = h$ for some value h. The table shows the second order convergence.

Table 1. Deviation between the exact values and computations by (17) in the discrete maximum norm.

$(k = 1, \quad v_0(x) = 6x(1 - x), \quad T = X_M = 1)$

	$\tau = h = 1/20 =$ $= 5 \cdot 10^{-2}$	$\tau = h = 1/40 =$ $= 2.5 \cdot 10^{-2}$	$\tau = h = 1/80 =$ $= 1.25 \cdot 10^{-2}$	$\tau = h = 1/120 \approx$ $\approx 8.33 \cdot 10^{-3}$
p=q=2	$3.44 \cdot 10^{-3}$	$8.61 \cdot 10^{-4}$	$2.15 \cdot 10^{-4}$	$9.56 \cdot 10^{-5}$
p=q=3	$2.61 \cdot 10^{-3}$	$6.35 \cdot 10^{-4}$	$1.59 \cdot 10^{-4}$	$7.05 \cdot 10^{-5}$
p=q=4	$2.37 \cdot 10^{-3}$	$5.88 \cdot 10^{-4}$	$1.47 \cdot 10^{-4}$	$6.53 \cdot 10^{-5}$

Table 2 contains the deviation of computed and exact solution in the discrete maximum norm if the initial function is noncontinuous. For the sake of comparison these deviations are also computed by (40) using the same parameters. These results are shown in Table 3. The computations have been made with $\tau = h$ and

$$\hat{v}_0(x) = \begin{cases} 0, & \text{if } 0 \leq x < 0.5, \\ 2, & \text{if } 0.5 \leq x \leq 1. \end{cases}$$

Table 2 shows the first order convergence and Table 3 shows the second order convergence.

Table 2. Deviation between the exact values and values computed from (17) in discrete maximum norm.

$$(k = 1, \quad v_0(x) = \hat{v}_0(x), \quad T = X_M = 1)$$

	$\tau = h = 1/20 =$ $= 5 \cdot 10^{-2}$	$\tau = h = 1/40 =$ $= 2.5 \cdot 10^{-2}$	$\tau = h = 1/80 =$ $1.25 \cdot 10^{-2}$	$\tau = h = 1/120 \approx$ $\approx 8.33 \cdot 10^{-3}$
p=q=2	$1.10 \cdot 10^{-1}$	$5.65 \cdot 10^{-2}$	$2.87 \cdot 10^{-2}$	$1.93 \cdot 10^{-2}$
p=q=3	$1.15 \cdot 10^{-1}$	$5.92 \cdot 10^{-2}$	$3.00 \cdot 10^{-2}$	$2.01 \cdot 10^{-2}$
p=q=4	$1.13 \cdot 10^{-1}$	$5.79 \cdot 10^{-2}$	$2.93 \cdot 10^{-2}$	$1.96 \cdot 10^{-2}$

Table 3. Deviation between the exact values and computations by (40) in the discrete maximum norm.

$$(k = 1, \quad v_0(x) = \hat{v}_0(x), \quad T = X_M = 1)$$

	$\tau = h = 1/20 =$ $= 5 \cdot 10^{-2}$	$\tau = h = 1/40 =$ $2.5 \cdot 10^{-2}$	$\tau = h = 1/80 =$ $1.25 \cdot 10^{-2}$	$\tau = h = 1/120 \approx$ $\approx 8.33 \cdot 10^{-3}$
p=q=2	$2.20 \cdot 10^{-3}$	$5.42 \cdot 10^{-4}$	$1.34 \cdot 10^{-4}$	$5.96 \cdot 10^{-5}$
p=q=3	$4.23 \cdot 10^{-3}$	$1.04 \cdot 10^{-3}$	$2.56 \cdot 10^{-4}$	$1.13 \cdot 10^{-4}$
p=q=4	$7.42 \cdot 10^{-3}$	$1.84 \cdot 10^{-3}$	$4.56 \cdot 10^{-4}$	$2.02 \cdot 10^{-4}$

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