SOLUTION OF A GENERAL POPULATION BALANCE EQUATION BY THE LAPLACE TRANSFORM AND PARTICLES FILTER TECHNIQUES

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Abstract. *The Laplace transform technique with numerical inversion was used to solve an integro-partial-differential equation related to the mathematical modeling of the physical problem to study convective processes with birth and death rates of particles or aerosols. Such model is governed by the population balance equation (PBE), in which is taken into account the nucleation, growth and coagulation processes. A Bayesian method was employed to solve the non-linear inverse problem and estimate the size distribution density function, thus predicting the dynamic behavior of the physical system. Specifically, the application of the particle filter with resampling algorithm has been applied as a method of solving the problem. From these solutions, numerical results were obtained and compared with those available in previous works in the literature permitting a critical evaluation of the present solution methodology*.

Keywords*: Population Balance Equation, Laplace transform, Numerical inversion, Particles filter*.

1. INTRODUCTION

The dynamic behavior of a population of small particles is a subject of interest in the fields of atmospheric physics, crystallization, and colloid chemistry. In all such systems, particles grow through collisions and coalescence with other particles (coagulation) and through accretion of material in the medium containing the particles (Ramabhadran et al., 1976). The mathematical description of system where nucleation, growth, and aggregation occur is referred to as the population balance (PB). The PB often takes the form of a nonlinear integro-partial-differential equation and rarely analytically tractable (Litster et al., 1995). Precipitation and crystallization are widely studied problems in modern chemical engineering. Several phenomena are involved, such as mixing at various scales, nucleation, crystal growth, aggregation, and breakage (Marchisio et al., 2003). The influence of mixing on this kind of process has been studied for more than two decades, leading to different and sometimes contradictory results (Baldyga et al., 1995; Barresi et al., 1999; Kim and Tarbell, 1996).

Particularly, for atmospheric aerosols, the most important phenomena are coagulation and heterogeneous condensation. Because of the strong dependence of aerosol properties such as scattering, on particle size, it is desirable to understand in as much details as possible how a size distribution evolves under the influence of the two processes. The size distribution of an aerosol is described by its size distribution density function, which is governed for a general population balance equation. For simulations of atmospheric aerosol dynamics including turbulence transport and dispersion, numerical solution of the equation will ultimately be necessary. However, analytical solutions for certain limiting cases of a spatially homogeneous can be valuable in understanding the qualitative structure of the behavior in more complex situation particles (Ramabhadran et al., 1976; Peterson et al., 1978; Gelbard and Seinfeld, 1978).

In this context, the objective this work is to obtain a solution via Laplace transform with numerical inversion and Bayesian filter with sampling importance resampling (SIR) filter for a general equation that governs the size distribution of particulates. The solution should be useful for describing the dynamic behavior of any system of particles which will be occurring coagulation and condensation. Also, analytical solutions for previously situations treated in the literature will be obtained in order to permit a critical comparison of the present solution methodology.

2. ANALYSIS

The spatial and chemical state of a homogeneous particulate system is described by the particle density function of the size distribution, n(v,t), where n(v,t)dv is the number of particles per unit volume of fluid in the range of volume v of v+dv. The drive for a similar system in which an individual particle may grow by adding material through the fluid phase (sink or loss of material), in which particles can collide and coagulate, are described by the general population balance equation (Ramabhadran et al., 1976; Drake, 1972) in the form:

$$\frac{\partial n(v,t)}{\partial t}=-\frac{\partial}{\partial v}\left[I(v,t)n(v,t)\right]+\frac{1}{2}\int_0^v \beta(v-\tilde{v},\tilde{v})n(v-\tilde{v},t)n(\tilde{v},t)d\tilde{v}-n(v,t)\int_0^\infty \beta(v,\tilde{v})n(\tilde{v},t)d\tilde{v}+S\left[n(v,t),v,t\right] \quad (1.a)$$

Where I(v,t) = dv/dt, is the change in the rate of volume of a particle of volume v for the transfer of material between the particles and fluid phase, $\beta(v,\tilde{v})$ is the coagulation coefficient for particles of volume v and $\tilde{v}$, S is the rate for net addition of new particles in the system. The initial and boundary conditions for Eq. (1.a) are usually given as:

$$n(v,0)=\frac{N_0}{v_0}e^{-v/v_0}; \quad n(0,t)=0 \quad (1.b,c)$$

The first term on the right side of Eq. (1) represents the growth rate of particles by mass transfer to individual particles. The second term represents the rate of accumulation of particles in the size range (v, v+dv) by the collision of two particles of volume $v-\tilde{v}$ and $\tilde{v}$ to form a particle of volume v (assuming conservation of volume during coagulation). The third term represents the rate of loss in the range of particle size (v, v+dv) by collision with all other particles. The last term represents all sources and sinks of particles. Equation (1) provides a wide variety of physical context, similar to colloid chemistry, atmospheric dynamics of aerosols, crystallization kinetics and biological population dynamics. In this paper, we will consider applications without the last term of Eq. (1.a), i.e., S[n(v,t),v,t] = 0.

2.1. Solution methodology via Laplace transform technique

For solving the mathematical model given by integro-partial-differential equation (1), the Laplace transform technique with numerical inversion was employed. Therefore, for this purpose, one test-case was considered: $\beta(v,\tilde{v})=\beta_0$ and I(v,t)=σv.

The Laplace transform procedure of Eq. (1.a), in order to remove the independent variable v is now established as follows:

$$\begin{aligned}&\mathcal{L}\left[\frac{\partial n(v,t)}{\partial t}\right]=\frac{\partial \bar{n}(s,t)}{\partial t};\ \mathcal{L}\left[\frac{\partial[\sigma v n(v,t)]}{\partial v}\right]=-\sigma s\frac{\partial \bar{n}(s,t)}{\partial s};\\ &\mathcal{L}\left[\frac{\beta_0}{2}\int_0^v n(v-\tilde{v},t)n(\tilde{v},t)d\tilde{v}\right]=\frac{\beta_0}{2}\bar{n}^2(s,t);\ \mathcal{L}\left[\beta_0 n(v,t)\int_0^\infty n(\tilde{v},t)d\tilde{v}\right]=\beta_0 M_0(t)\bar{n}(s,t)\end{aligned} \quad (2.a\text{-}d)$$

where, $\bar{n}(s,t)=\mathcal{L}[n(v,t)]$.

Therefore, the transformed differential equation, from the results of Eqs. (2), together with the transformed initial condition, are written as

$$\frac{\partial \bar{n}(s,t)}{\partial t}-\sigma s\frac{\partial \bar{n}(s,t)}{\partial s}=\frac{\beta_0}{2}\bar{n}^2(s,t)-\beta_0 M_0(t)\bar{n}(s,t); \quad \bar{n}(s,0)=\frac{(N_0/v_0)}{s+(1/v_0)} \quad (3.a,b)$$

The zeroth order moment $M_0(t)$ that appears in Eq. (3.a) is obtained from the its usual definition, and for this case is given by (Ramabhadran et al., 1976)

$$M_0(t)=\int_0^\infty n(v,t)dv=\frac{2N_0}{2+\beta_0 N_0 t} \quad (3.c)$$

Equation (3.a) is also analytically solved through the method of characteristics, to yield

$$\bar{n}(s,t)=\frac{4(N_0/v_0)e^{-\sigma t}}{(2+\beta_0 N_0 t)^2\{s+2e^{-\sigma t}/[(2+\beta_0 N_0 t)v_0]\}} \quad (4)$$

where, $\tau=\beta_0 \mathrm{N}_0 t$, $\Lambda=\sigma/\beta_0\mathrm{N}_0=1.0$, $D_0=1$ and $v_0=1$

$$\bar{n}(s,t)=\frac{4(N_0/v_0)e^{-\Lambda\tau}}{(2+\tau)^2\{s+2e^{-\Lambda\tau}/[(2+\tau)v_0]\}} \quad (5)$$

Assuming spherical particles, the volume distribution density is now related to its diameter distribution density through

$$n_D(D,t) = \frac{\pi D^2}{2} n(v,t) \tag{6}$$

$$v_0 = \frac{D_0{}^3 \pi}{6}; \bar{n}_D(\bar{D},t) = D_0 n_D(D,t) \tag{7.a,b}$$

2.2. The particle filter

The particle filter is a numerical method of integration, it is suitable to solve nonlinear and not Gaussian problems. Since the sixties, considerable attention has been devoted to these problems. However, only with increased computing power could make it more usual.

Many problems in science require state estimation for a system in which changes over time using a sequence of noise measurements are made over the system. Thus, differential equations are used to model the evolution of the system over time, and measurements are taken to assess the discrete moments. To estimate the dynamic state, the discrete time approach is generalized and convenient (Arulampalam et al, 2002).

The algorithm of sequential importance sampling (SIS) is a Monte Carlo (MC) method which forms the basis for most sequential MC filters developed over the past decades. This sequential approach MC (SMC) is also known as bootstrap filtering, interacting particle approximations and survival of the fittest. It is a technique for implementing a recursive Bayesian filter by MC simulations. The key idea is to represent the required posterior density function by a set of random samples with associated weights and calculate the estimates based on these samples and weights. This characterization MC becomes an equivalent representation to the usual functional description of the posterior probability density function (pdf). As the number of samples becomes very large approaches such as the SIS filter is an optimal Bayesian estimation (Arulampalam et al., 2002).

We present below the so-called Sequential Importance Sampling (SIS) algorithm for the particle filter, which includes a resampling step at each instant, as described in detail in Arulampalam et al. (2002). The SIS algorithm makes use of an importance density, which is a density proposed to represent another one that cannot be exactly computed, that is, the sought posterior density in the present case. Then, samples are drawn from the importance density instead of the actual density.

Let $\{x_{0:k}^i, i = 0,...,N\}$ be the particles with associated weights $\{w_k^i, i = 0,...,N\}$ and $x_{0:k} = \{x_j, j = 0,...,k\}$ be the set of all states up to t_k, where N is the number of particles. The weights are normalized so that $\sum_{i=1}^{N} w_k^i = 1$. Then, the posterior density at t_k can be discretely approximated by (Orlande et al., 2008):

$$\pi(x_{0:k} | z_{1:k}) \approx \sum_{i=1}^{N} w_k^i \delta(x_{0:k} - x_{0:k}^i) \tag{8}$$

where δ(.) is the Dirac delta function. The evolution-observation model is based on the following assumptions (Kaipio and Somersalo, 2004; Kaipio et al., 2005):

(i) The sequence x_k for k = 1, 2, …, is a Markovian process, that is

$$\pi(x_k | x_0, x_1, ..., x_{k-1}) = \pi(x_k | x_{k-1}) \tag{9}$$

(ii) The sequence z_k for k = 1, 2, …, is a Markovian process with respect to the history x_k, that is

$$\pi(z_k | x_0, x_1, ..., x_{k-1}) = \pi(z_k | x_{k-1}) \tag{10}$$

(iii) The sequence x_k depends on the past observation only through its own history, that is

$$\pi(x_k | x_{k-1}, z_{1:k-1}) = \pi(x_k | x_{k-1}) \tag{11}$$

By taking hypotheses (7-9) into account, the posterior density (6) can be written as (Arulampalam et al., 2002):

$$\pi(x_k | z_k) \approx \sum_{i=1}^{N} w_k^i \delta(x_k - x_k^i) \tag{12}$$

A common problem with the SIS particle filter is the degeneracy phenomenon, where after a few states all but one particle will have negligible weight (Kaipio and Somersalo, 2004; Kaipio et al., 2005; Arulampalam et al., 2002; Orlande et al., 2008). This degeneracy implies that a large computational effort is devoted to updating particles whose contribution to the approximation of the posterior density function is almost zero. This problem can be overcome by increasing the number of particles, or more efficiently by appropriately selecting the importance density as the prior density $\pi(x_k \left| x_{k-1}^i \right.)$. In addition, the use of the resampling technique is recommended to avoid the degeneracy of the particles.

Resampling involves a mapping of the random measure $\{x_k^i, w_k^i\}$ into a random measure $\{x_k^{i*}, N^{-1}\}$ with uniform weights. It can be performed if the number of effective particles with large weights falls below a certain threshold number. Alternatively, resampling can also be applied indistinctively at every instant t_k, as in the Sampling Importance Resampling (SIR) algorithm described in (Arulampalam et al., 2002; Orlande et al., 2008). Such algorithm can be summarized in the following steps, as applied to the system evolution from t_{k-1} to t_k (Arulampalam et al., 2002; Orlande et al., 2008):

Step 1. For i=1,…, N draw new particles x_k^i from the prior density $\pi(x_k \left| x_{k-1}^i \right.)$ and then use the likelihood density to calculate the correspondent weights $w_k^i = \pi(z_k \left| x_k^i \right.)$.

Step 2. Calculate the total weight $T_w = \sum_{i=1}^{N} w_k^i$ and then normalize the particle weights, that is, for i=1,…, N let $w_k^i = T_w^{-1} w_k^i$.

Step 3. Resample the particles as follows:

Step 3.1. Construct the cumulative sum of weights (CSW) by computing $c_i = c_{i-1} + w_k^i$ for i = 1,…, N, with $c_0 = 0$.

Step 3.2. Let i = 1 and draw a starting point u_1 from the uniform distribution $U[0, N^{-1}]$.

Step 3.3. For j = 1,…,N

– Move along the CSW by making $u_j = u_{j-1} + N^{-1}(j-1)$.
– While $u_j > c_i$ make i = i +1.
– Assign sample $x_k^j = x_k^i$.
– Assign weight $x_k^j = N^{-1}$.

Although the resampling step reduces the effects of the degeneracy problem, it may lead to a loss of diversity and the resultant sample can contain many repeated particles. This problem, known as sample impoverishment, can be severe in the case of small process noise. In this situation, all particles collapse to a single particle within few instants t_k (Kaipio and Somersalo, 2004; Arulampalam et al., 2002; Orlande et al., 2008). Another drawback of the particle filter is related to the large computational cost due to the Monte Carlo method, which may limit its application to complicated physical problems.

3. RESULTS AND DISCUSSION

Numerical results for the diameter distribution density were obtained. For this purpose, computer codes were developed in the Fortran 90/95 programming language, which were run on a Intel (R) CORE i3 2.13 GHz computer. For the numerical inversion of Eq. (5), the subroutine DINLAP from the IMSL (1991) Library was used with a tolerance of 10^{-4}. The SIR filter was used to estimate [n(v,t)], with the number of particles (Np = 500, 1000 and 2000) for the estimated state variables, the RMS error (square root of the mean square error) by Eq. (13) is shown in Tables (1) to (3) in the range from 10^{-5} to 10^{-6}. We analyzed the standard deviation (σ) of the model (σmodel) and measures (σmeasures) of 1% and 5%, which were tested with the combinations (σmeasures = 0.01 and σmodel = 0.05, σmeasures = 0.05 and σmodel = 0.01). The combinations are shown in the Tables (1) to (3) for times τ = 0.5, 1.0 and 2.0, and in Fig. 1.a and 1.b for times τ = 2.0. Such results were compared with measurements (measured value plus a random value multiplied by the standard deviation of measurements) of the particulate filter.

$$\mathrm{eRMS} = \sum_{i=1}^{Nt} \sum_{j=1}^{Np} \frac{\left(C_{exato,i,j} - C_{estimado,i,j}\right)^2}{Nt * Np} \qquad (13)$$

Table 1. eRMS for the test-case and τ = 0.25

σmeasures - σmodel	Np = 500	Np = 1000	Np = 2000
0.01 – 0.05	3.096E-6	2.451E-6	3.050E-6
0.05 – 0.01	5.881E-5	5.666E-5	3.752E-5

Table 2. eRMS for the test-case and τ = 1.0

σmeasures - σmodel	Np = 500	Np = 1000	Np = 2000
0.01 – 0.05	3.617E-6	2.746E-6	2.704E-6
0.05 – 0.01	5.423E-5	5.872E-5	9.988E-5

Table 3. eRMS for the test-case and τ = 2.0

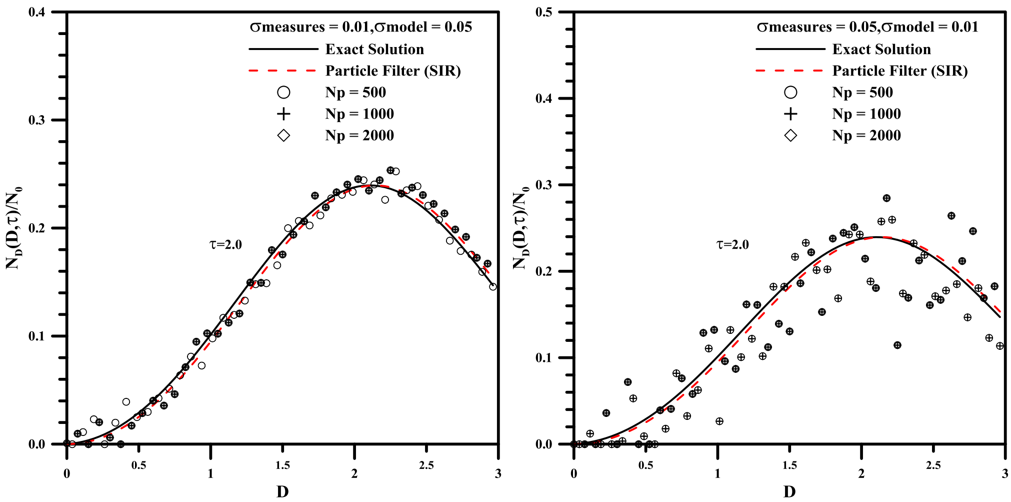
σmeasures - σmodel	Np = 500	Np = 1000	Np = 2000
0.01 – 0.05	2.890E-6	3.515E-6	2.927E-6
0.05 – 0.01	5.114E-5	5.154E-5	6.156E-5

Figures 1 show the behavior of the measurements for Np = 500, 1000 and 2000 which were compared with the exact solution and SIR filter results for the time τ = 2.0. It is observed that the results have graphically a good convergence within the standard deviation. From this point on, it was adopted a number of particles Np = 1000 to estimate the density function in all cases, since no difference was observed in the results increasing the numbers of particles.

Figures 2 show the graphical comparisons between the results of exact solution with those obtained via the SIR filter for τ = 0.25. In Fig. 2.a is noted that the measures converge to the values measured when the standard deviation is in the range 0.01 to 0.05. Also, it is observed that the measures and the estimated values are within the confidence interval 99% of the model. Analyzing Fig. 2.b, it notes that the measures fall short of the measured values and try to get the results estimated when the standard deviation is large (0.05 - 0.01), also one can see that the measured and estimated values are partially outside confidence interval 99% of the model.

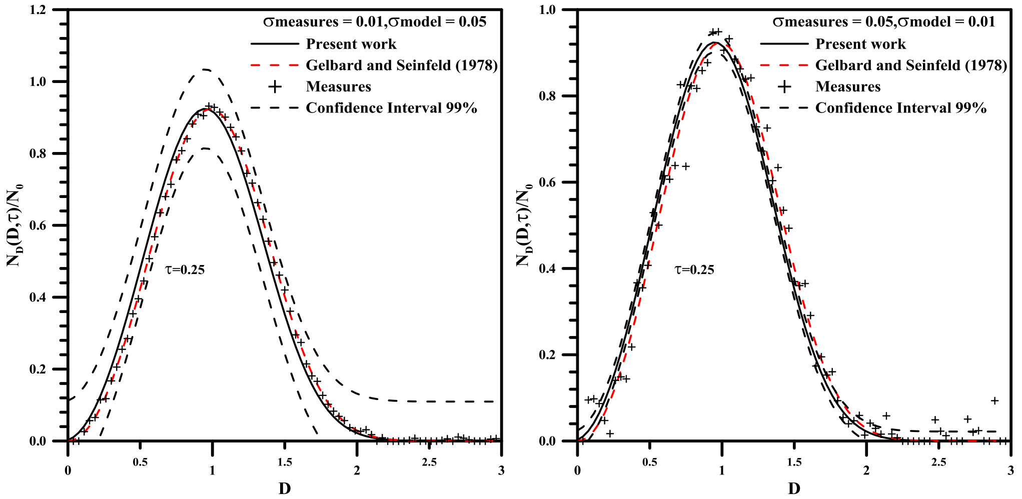
In Figs. 3.a and 3.b, it is shown the graphical comparisons between the results of exact solution with those obtained via SIR filter for τ = 1.0. It is noted from Fig. 3.a that the measures tend to standard deviation values measured for the large model, which are within confidence interval 99%. Figure 3.b shows that the measures leave the measured values and try to get the model, but for small values of the density function, it results in sharp fluctuations in the measurements.

Finally in Figs. 4, it is shown the graphical comparisons between the results of exact solution with those obtained via the particle filter (SIR) for τ = 2.0. It is observed in Fig. 2.a that measures tend to the values measured for small standard deviation of the measured values which are within confidence interval 99%. Also it is noted in Fig. 2.b that measures have strong oscillations and abandon the measured values for large standard deviation measures and try to converge to the model.



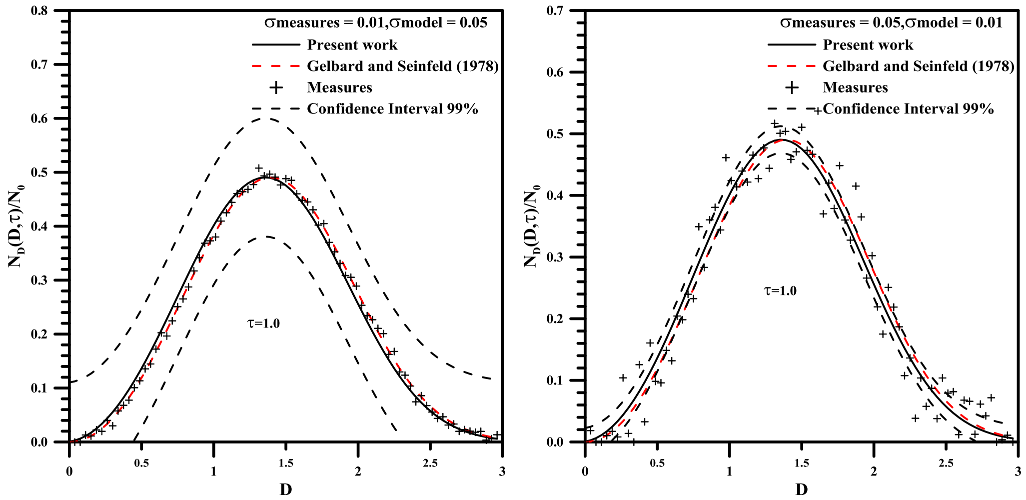
(a) (b)

Figure 1. Behavior of the exact solution with SIR filter for τ = 2.0. (a) σmeasures = 0.01 and σmodel = 0.05; (b) σmeasures = 0.05 and σmodel = 0.01.



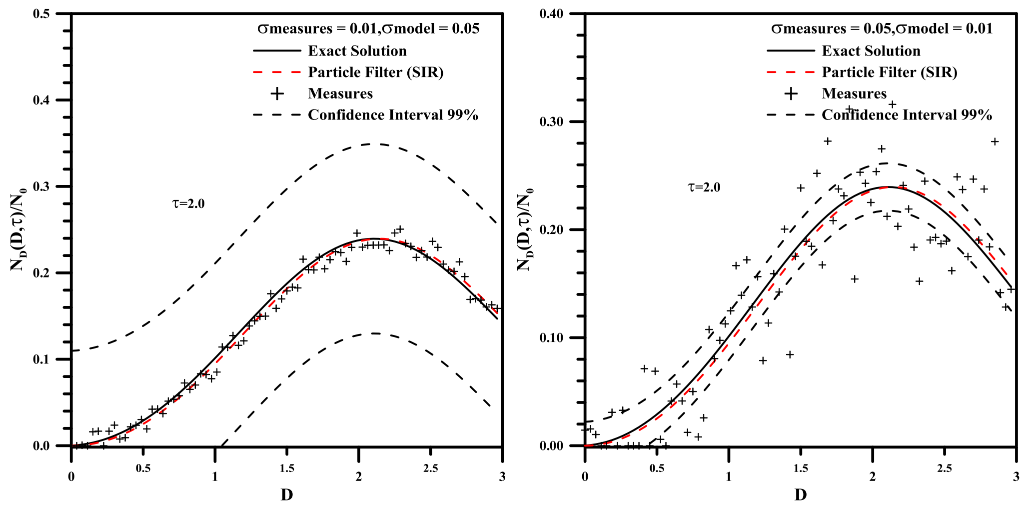
(a) (b)

Figure 2. Comparison of the inverse Laplace solution with SIR filter for τ = 0.25. (a) σmeasures = 0.01 and σmodel = 0.05; (b) σmeasures = 0.05 and σmodel = 0.01.



(a) (b)

Figure 3. Comparison of the inverse Laplace solution with SIR filter for τ = 1.0. (a) σmeasures = 0.01 and σmodel = 0.05; (b) σmeasures = 0.05 and σmodel = 0.01.



(a) (b)

Figure 4. Comparison of the inverse Laplace solution with SIR filter for τ = 2.0. (a) σmeasures = 0.01 and σmodel = 0.05; (b) σmeasures = 0.05 and σmodel = 0.01.

4. CONCLUSIONS

In this work it was shown the applicability of the Laplace transform technique with numerical inversion in the solution of population balance equation as test-case. We used the subroutine DINLAP from the IMSL Library (1991) which performs the numerical inversion of the Laplace transform and the results generated were compared with data produced by the analytical solution, which have excellent agreement. Analyzing the behavior of the graphs generated in this study, we conclude that the Laplace transform technique with numerical inversion is an alternative tool in solving the problems studied. The Bayesian filter used in this study was the Sampling and Importance Resampling (SIR) Sequential filter, which was applied to a hyperbolic and nonlinear problem represented by the PBE, in order to estimate the density function of particle size, which demonstrated to be able to estimate such density function.

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