**Int. j. adv. multidisc. res. stud.** 2026; 6(2):1275-1280

**Received:** 19-02-2026
**Accepted:** 29-03-2026

International Journal of Advanced Multidisciplinary Research and Studies

ISSN: 2583-049X

# Numerical Solution and Stability Analysis of the Modified Linear Adsorption Model for Nanoparticles Transport in Porous Media Using the Crank-Nicolson Method

**[1] Umeshkumar C Prajapati, [2] MR Tailor**
[1] Department of Mathematics, RNGPIT, Isroli, Bardoli, Surat, Gujarat, India
[2] Department of Mathematics, Patidar Gin Science College, Bardoli, Surat, Gujarat, India

Corresponding Author: **Umeshkumar C Prajapati**

## Abstract

The transport and retention of nanoparticles in porous media are essential processes that impact the outcomes of Enhanced Oil Recovery (EOR). A Modified Linear (ML) adsorption model was formulated to examine nanoparticle transport using a simplified linear association between adsorbed and aqueous concentrations, resulting in a modified advection-dispersion equation that includes an effective retention term. This study reformulates and resolves the modified linear model applying the Crank-Nicolson finite difference method. All physical and numerical parameters are derived directly from literature related to four fundamental flood research studies employing coated silica and iron oxide nanoparticles in Boise sand packs. The research confirms that the Modified Linear Model, discretised by Crank-Nicolson, accurately represents the delayed breakthrough, plateau behaviour, and post-flush decrease observed in experiments, showing consistent numerical performance.

**Keywords:** Nanoparticle Transport, Modified Linear Adsorption Model, Crank Nicolson Scheme, Porous Media, Enhanced Oil Recovery

## 1. Introduction

Nanotechnology has shown potential for application in both the upstream and downstream segments of petroleum production in recent years Bera and Belhaj [3]. An effective study has been conducted on the application of nanotechnology in numerous industries, with a focus on Enhanced oil recovery (EOR). The efficiency of oil recovery from reservoirs has increased due to the capacity of nanoparticle-sized particles to penetrate micropore throats and interact chemically or physically with the reservoir fluid-rock system [3]. One of the most promising materials is silica-based nanoparticles (NPs) because of their simplicity of engineering and manufacture [6, 12, 13].

Nano enhanced oil recovery (nano EOR) fundamentally depends on a quantitative comprehension of nanoparticle migration and retention in porous media, as adsorption and deposition processes directly influence nanoparticle deliverability and the formation of surface attachment layers that can alter rock wettability [2, 7]. Experimental and theoretical investigations indicate that nanoparticle deposition is influenced by several interacting parameters, such as pore-scale velocity, particle and grain dimensions, pH, ionic strength, and temperature [9, 14, 17]. Unlike micron-scale colloids, which are primarily influenced by interception and gravitational settling, nanoparticles have significantly more intricate transport dynamics, with Brownian diffusion and electrostatic interactions being significant factors [3, 4].

The advection dispersion equation (ADE) is extensively utilised to characterise particle transport in porous media [5]. Nonetheless, when utilised in its traditional passive-tracer format, the ADE inadequately represents the critical deposition and retention processes linked to nanoparticle transport. To reduce this limitation, additional reaction or retention terms must be integrated to account for particle adhesion to pore surfaces [16]. Multiple deposition models have been suggested for this objective, including colloidal filtration theory (CFT) and its extensions, kinetic Langmuir-type models, and dual-site adsorption formulations [8, 10, 15]. While these methodologies can enhance physical realism, their practical implementation can often be delayed by the challenge of determining many model parameters, especially in dual-site setups.

The modified linear adsorption model (ML) aims to combine physical accuracy with mathematical and computational simplicity by suggesting a linear equilibrium relationship between the concentration of movable nanoparticles and the surface-associated concentration, defined by a concentration distribution coefficient and single-collector efficiency [11]. This formulation preserves the essential advantages of adsorption while upholding a linear governing partial differential equation, rendering it suitable for dependable and efficient numerical solutions. This study develops a Crank Nicolson finite-difference

scheme to solve the modified linear model, replicate effluent concentration histories aligned with previously reported ML results, and systematically evaluate the numerical performance of the method regarding stability, accuracy, and convergence.
Several models that have been developed for nanoparticle transport were studied. Based on that, we proposed a Modified Linear Adsorption model. Experimental data from Madhan Nur Agista [1] was used to validate the model.

## 2. Background

This section develops the governing equation used in the simulation, showing the transition from the constitutive relationships to the final partial differential equation.

### 2.1 A Summary of the Numerical Study

Analyse the representative elementary volume (REV) of the porous medium. The conservation of mass for nanoparticles requires that the mass accumulation within the representative elementary volume (REV) be equal to the net inflow minus the net discharge, along with any reaction sources or sinks (deposition).

$$\frac{\partial C}{\partial t}+\frac{\rho_b}{\phi}\frac{\partial s}{\partial t}=D\frac{\partial^2 C}{\partial x^2}-v\frac{\partial C}{\partial x} \tag{1}$$

This is the general form of the ADE with a reaction term. The term $\frac{\rho_b}{\phi}\frac{\partial s}{\partial t}$ represents the transfer of mass from the aqueous phase to the solid rock surface.

### 2.2 Modified Linear Adsorption

In this study, we suggested a simplified modified linear adsorption model to provide a fundamental understanding of the adsorption of NP on solid surfaces. The model considers that the concentration of particles on the solid surface ($s$) is linear to the concentration of particles inside the fluid ($C$), with their relationship expressed in equations (2) and (3).

$$s = k_c C\eta_o \tag{2}$$

$$\frac{\partial s}{\partial t}=k_c\,\eta_o\frac{\partial C}{\partial t} \tag{3}$$

Where Distribution Coefficient $k_c$: the concentration distribution coefficient of NP between solid and fluid phases.
Collector Efficiency $\eta_o$: A transport parameter indicating the probability that a particle approaching a grain would come into contact with it.
To integrate this into the mass balance, we compute the time derivative of Equation (2). Assuming that $k_c$ and $\eta_o$ are constants for a specific flow system (steady-state velocity and temperature):
This indicates that adsorption occurs quickly and is reversible. If $C$ rises, $s$ rises instantly. Significantly, if $C$ decreases (as observed in a post-flush situation), $s$ immediately decreases, releasing particles back into the fluid.
Substituting Equation (3) into the general ADE Equation (1):

$$\frac{\partial C}{\partial t}+\frac{\rho_b}{\phi}\left(k_c\eta_o\frac{\partial C}{\partial t}\right)=D\frac{\partial^2 C}{\partial x^2}-v\frac{\partial C}{\partial x} \tag{4}$$

Equation (4) become

$$\left(1+\frac{\rho_b}{\phi}k_c\eta_o\right)\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}-v\frac{\partial C}{\partial x} \tag{5}$$

This is the equation that governs the solution. The term within the brackets is dimensionless and is commonly known as the Retardation Factor $R$ in hydrogeology:

$$R=1+\frac{\rho_b}{\phi}k_c\eta_o \tag{6}$$

Equation (5) become:

$$R\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}-v\frac{\partial C}{\partial x} \tag{7}$$

The initial conditions the domain is initially free of nanoparticles.

$$C(x,0)=0,\ \ s(x,0)=0 \quad \text{for } 0\le x\le L \tag{8}$$

The boundary conditions are:

Inlet Boundary ($\boldsymbol{x = 0}$): A finite slug of nanofluid is injected. The concentration is $C_o$ for a specific duration $t_{slug}$ followed by a brine flush $(C = 0)$. This is a Dirichlet condition that varies with time.

$$c(0,t) = \begin{cases} c_o & \text{if } 0 \le t \le t_{slug} \\ 0 & \text{if } t > t_{slug} \end{cases} \tag{9}$$

Outlet Boundary **($\boldsymbol{x = L}$):** We assume the concentration gradient becomes negligible at the outlet, allowing particles to flow out freely without accumulation. This is a Neumann condition.

$$\frac{\partial C}{\partial x}(L,t) = 0 \quad \text{for } t > 0 \tag{10}$$

## 3. Numerical Solution of Modified Linear Model

The system Eq. (7)-(10) is solved using Crank Nicolson method

Substitute $\frac{\partial C}{\partial t}, \frac{\partial^2 C}{\partial x^2}$ *and* $\frac{\partial C}{\partial x}$ in equation (7):

$$\frac{\partial C}{\partial t} = \frac{C_{i,j+1} - C_{i,j}}{\Delta t}, \frac{\partial C}{\partial x} = \frac{(C_{i+1,j+1} - C_{i-1,j+1}) + (C_{i+1,j} - C_{i-1,j})}{4(\Delta x)},$$
$$\frac{\partial^2 C}{\partial x^2} = \frac{(C_{i+1,j+1} - 2C_{i,j+1} + C_{i-1,j+1}) + (C_{i+1,j} - 2C_{i,j} + C_{i-1,j})}{2(\Delta x)^2}, \tag{11}$$

Equation (9) becomes,

$$(R)\left(\frac{C_{i,j+1} - C_{i,j}}{\Delta t}\right) = D\left(\frac{(C_{i+1,j+1} - 2C_{i,j+1} + C_{i-1,j+1}) + (C_{i+1,j} - 2C_{i,j} + C_{i-1,j})}{2(\Delta x)^2}\right)$$
$$- v\left(\frac{(C_{i+1,j+1} - C_{i-1,j+1}) + (C_{i+1,j} - C_{i-1,j})}{4(\Delta x)}\right) \tag{12}$$

$$(R)\left(\frac{C_{i,j+1} - C_{i,j}}{1}\right) = D(\Delta t)\left(\frac{(C_{i+1,j+1} - 2C_{i,j+1} + C_{i-1,j+1}) + (C_{i+1,j} - 2C_{i,j} + C_{i-1,j})}{2(\Delta x)^2}\right)$$
$$- v(\Delta t)\frac{(C_{i+1,j+1} - C_{i-1,j+1}) + (C_{i+1,j} - C_{i-1,j})}{4(\Delta x)} \tag{13}$$

$$-(\alpha + \beta)C_{i-1,j+1} + (1 + 2\alpha)C_{i,j+1} + (-\alpha + \beta)C_{i+1,j+1} =$$
$$(\alpha + \beta)C_{i-1,j} + (1 - 2\alpha)C_{i,j} + (\alpha - \beta)C_{i+1,j} \tag{14}$$

Where;

$$\alpha = \frac{D\Delta t}{2R(\Delta x)^2}, \quad \beta = \frac{v\Delta t}{4R\Delta x}, i = 1 \; to \; N + 1, and \; j = 0 \; to \; N - 1 \tag{15}$$

This system is solved at every time step using the Thomas Algorithm, which is computationally efficient for tridiagonal systems.

### 3.1 Collected Experiments and Measurements

We use experimental data sets from the literature (Agista, 2017, citing Murphy, 2012) to test the Modified Linear (ML) adsorption numerical model. These experiments investigated the transport of surface-coated nanoparticles through Boise sandstone packs. Two distinct types of nanoparticles were used to capture different transport regimes:

Experiments 66 and 67 (Silica Nanoparticles): In these experiments, 15 nm silica nanoparticles were coated with a polymer to make them more stable in brine with high salinity. Experiment 66 was conducted at a high flow rate of 10 cc/min, while Experiment 67 was conducted at a low flow rate of 1 cc/min. The change in velocity makes it possible to test rate-dependent retention effects.

Experiments 91 and 92 (Iron Oxide Nanoparticles): These tests used iron oxide (magnetite) nanoparticles that were 150 nm in size. These were done at low (1 cc/min) and high (8.4 cc/min) flow rates, just like the silica experiments. Iron oxide particles usually have different surface charge properties and Hamaker constants than silica, which makes them a good way to test the model's usefulness, particularly in understanding how these differences affect their behaviour in various environments and applications.

Table 1 of the source document lists the parameters that are needed for the numerical simulation. The parameters contain the physical characteristics of the porous media and the determined coefficients for the modified linear model.

**Table 1:** Simulation Parameters for Modified Linear Model

| Parameter (Unit) | Symbol | Exp 66 | Exp 67 | Exp 91 | Exp 92 |
|---|---|---|---|---|---|
| Pore Velocity (m/s) | $v$ | $3.70 \times 10^{-3}$ | $3.70 \times 10^{-4}$ | $3.80 \times 10^{-4}$ | $3.10 \times 10^{-3}$ |
| Dispersion Coefficient (m²/s) | $D$ | $8.80 \times 10^{-6}$ | $4.50 \times 10^{-7}$ | $3.20 \times 10^{-7}$ | $2.10 \times 10^{-6}$ |
| Single Collector Efficiency | $\eta_p$ | $6.57 \times 10^{-3}$ | $3.18 \times 10^{-2}$ | $9.71 \times 10^{-3}$ | $2.44 \times 10^{-3}$ |
| Distribution Coefficient | $k_c$ | $1.50 \times 10^{-2}$ | $4.00 \times 10^{-3}$ | $6.00 \times 10^{-2}$ | $1.35 \times 10^{-1}$ |
| Injected Pore Volume (PV) | PVI | 3.0 | 3.0 | 2.9 | 3.1 |
| Porosity | $\phi$ | 0.476 | 0.479 | 0.464 | 0.473 |
| Observed Recovery | $R_{exp}$ | 0.84 | 0.83 | 0.47 | 0.79 |
| Simulated Recovery | $R_{sim}$ | 0.81 | 0.82 | 0.43 | 0.75 |
| Relative Error (%) | $\varepsilon$ | 3.8% | 1.4% | 7.8% | 5.1% |

## 4. Results and Discussion

The simulation findings provide an entire view of how nanoparticles transport through porous media, proving that the Modified Linear (ML) model works better than traditional techniques for coated silica nanoparticles in Boise sandstone.

### 4.1 Analysis of Silica Nanoparticle Transport

Figure 1 shows the temporal evolution of the effluent concentration for Experiments 66 and 67 (Silica NPs). The figure shows the experimental data points, the tracer curve (a representation of non-reactive transport), and the Modified Linear (ML) simulation outcomes.

Temporal Evolution: In both velocity regimes, the experimental breakthrough of nanoparticles has been delayed in comparison to the tracer. This delay shows adsorption-induced retardation. the Modified Linear (ML) model, using the Crank-Nicolson method, effectively approximates this change in behaviour.

Experiment 66 (High Velocity): The simulation curve rises sharply, reflecting the experimental data. The model predicts an increased concentration slightly below $C/C_0 = 1.0$, suggesting the presence of irreversible loss or equilibrium partitioning. The match is strong during the injection phase.

Experiment 67 (Low Velocity): The delay increases because a lower velocity permits increased time spent for interaction, as seen by the velocity-dependent single collector efficiency $\eta_0$. the Modified Linear (ML) model identifies the "early peak" phenomenon evident in the data.

The agreement between the ML model and experimental data is remarkable, with relative errors in the total recovery of merely,3.8 % and 1.4 %, respectively. This indicates that the assumption of linear reversible adsorption for surface-modified silica nanoparticles in sandstone is physically valid. The slight variation in the post-flush tailing (desorption phase) indicates that while adsorption is largely reversible, the kinetics might be slightly rate-limited, resulting in a "smearing" of the trailing edge that the instantaneous equilibrium model represents as a more sharp drop.

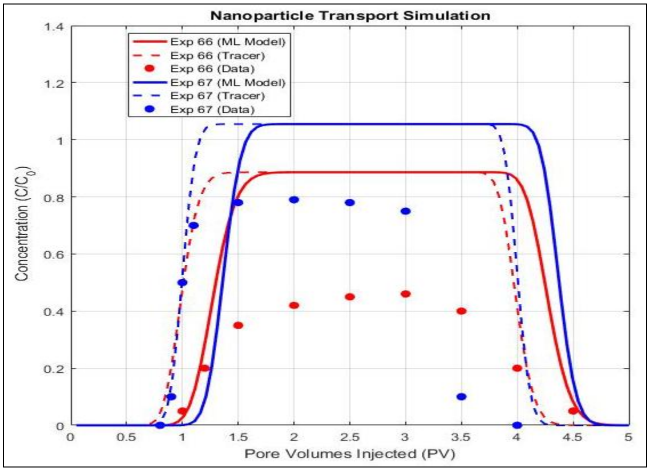

**Fig 1:** Effluent data and simulations that use Modified Linear (ML) results from tests 66 and 67

### 4.2 Analysis of Iron Oxide Nanoparticle Transport

Figure 2 shows the results of Experiments 91 and 92 (Iron Oxide Nanoparticles). This dataset shows how iron oxides' surface chemistry affects how they behave in detail.

Experiment 92 (High Velocity): The modified linear model shows that the breakthrough time and the rising part of the concentration curve are almost perfectly correlated. The Crank-Nicolson method effectively manages the steep front without generating numerical oscillations, thereby validating its stability. The recovery error is very small, only 5.1%.

Experiment 91 (Low Velocity): This experiment works as an important test in the case. The experimental recovery was minimal (47%), showing significant retention. The CFT model, examined in previous studies, drastically underestimated recovery by over 50% in this case due to its failure to appropriately incorporate finite capacity or retardation effects.

Figure 2 indicates that the modified linear model predicts a minor postponed breakthrough in relation to the experimental findings for Exp 91. This discrepancy suggests that for very low velocities, the assumption of a constant distribution coefficient may be too basic. The interaction may involve non-linear effects (e.g., Langmuir saturation) or kinetic rate restrictions that become relevant when the transport duration approximates the reaction duration (Damkohler number effects). The ability to assess overall behaviour when alternative models have not performed well illustrates the adaptability of the retardation factor approach.

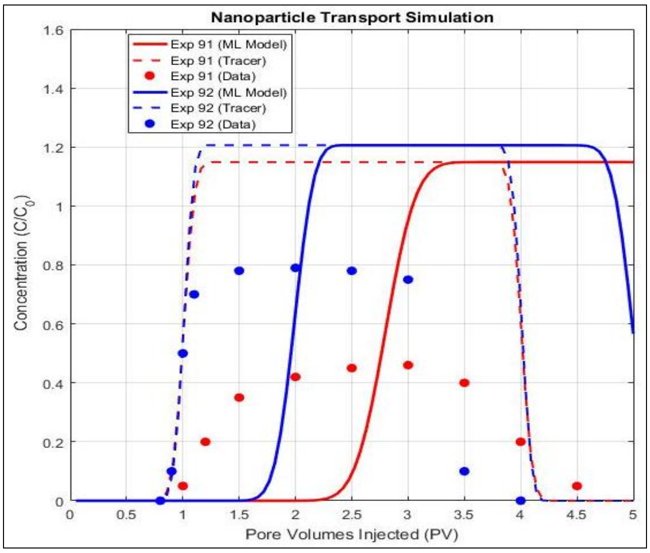

**Fig 2:** Effluent data and simulation applying Modified Linear (ML) results from experiments 91 and 92

## 5. Conclusion

This study has systematically studied the numerical solution of the modified linear adsorption model for nanoparticle transport in porous media. Applying the Crank-Nicolson finite difference method, we have successfully analysed the transport behaviour of silica and iron oxide nanoparticles under various flow conditions.

The modified linear model, denoted by equation (5), effectively captures the retardation and dispersion phenomena that predicate nanoparticle behaviour. It considerably improves conventional Colloidal Filtration Theory (CFT) in predicting effluent trajectories, reducing prediction errors from over 50% to approximately 8% in challenging low-recovery scenarios.

The research indicates that in the examined systems, nanoparticle retention is primarily affected by reversible interactions, which can be represented using a linear retardation factor. However, inefficiencies at low velocities indicate that future models may require the integration of rate-dependent kinetic parameters or non-linear isotherms.

The current research has methodically examined the numerical solution of the modified linear adsorption model for nanoparticle transport in porous media. Using the Crank-Nicolson finite difference method, we have successfully simulated the transport behaviour of silica and iron oxide nanoparticles under various flow conditions.

## 6. References

1. Madhan Nur Agista, P°al Østebø Andersen and Zhixin Yu. Modelling nanofluid injections in porous media. Journal of Petroleum Science and Engineering. 2019; 176:836-849.
2. Sarmad Al-Anssari, Ahmed Barifcani, Shaobin Wang, Lebedev Maxim, Stefan Iglauer. Wettability alteration of oil-wet carbonate by silica nanofluid. Journal of Colloid and Interface Science. 2016; 461:435-442.
3. Achinta Bera, Hadi Belhaj. Application of nanotechnology by means of nanoparticles and nano dispersions in oil recovery-a comprehensive review. Journal of Natural Gas Science and Engineering. 2016; 34:1284-1309.
4. Menachem Elimelech, Charles R O'Melia. Kinetics of deposition of colloidal particles in porous media. Environmental Science & Technology. 1990; 24(10):1528-1536.
5. David L Freyberg. A natural gradient experiment on solute transport in a sand aquifer: 2. spatial moments and the advection and dispersion of nonreactive tracers. Water Resources Research. 1986; 22(13):2031-2046.
6. Luky Hendraningrat. Unlocking the potential of hydrophilic nanoparticles as novel enhanced oil recovery method: An experimental investigation, 2015.
7. Luky Hendraningrat, Torsæter O. Understanding fluid-fluid and fluid-rock interactions in the presence of hydrophilic nanoparticles at various conditions. In SPE Asia Pacific Oil and Gas Conference and Exhibition, SPE 2014, SPE-171407.
8. Shidong LI. An experimental investigation of enhanced oil recovery mechanisms in nanofluid injection process, 2016.
9. Yusong LI, Yonggang Wang, Kurt D Pennell, Linda M Abriola. Investigation of the transport and deposition of fullerene (c60) nanoparticles in quartz sands under varying flow conditions. Environmental Science & Technology. 2008; 42(19):7174-7180.

10. Xueying Liu, Denis M O'Carroll, Elijah J Petersen, Qingguo Huang, Lind-say Anderson C. Mobility of multiwalled carbon nanotubes in porous media. En-vironmental Science & Technology. 2009; 43(21):8153-8158.
11. Francesca Messina, Daniele Luca Marchisio, Rajandrea Sethi. An extended and total flux normalized correlation equation for predicting single-collector efficiency. Journal of Colloid and Interface Science. 2015; 446:185-193.
12. Cigdem O Metin, Jimmie R Baran, Quoc P Nguyen. Adsorption of surface functionalized silica nanoparticles onto mineral surfaces and decane/water interface. Journal of Nanoparticle Research. 2012; 14:1-16.
13. Caetano Rodrigues Miranda, Lucas Stori de Lara, Bruno Costa Tonetto. Stability and mobility of functionalized silica nanoparticles for enhanced oil recovery applications. In SPE international oilfield nanotechnology conference and exhibition, SPE, 2012, SPE-157033.
14. Vasiliki I Syngouna, Constantinos V Chrysikopoulos. Interaction between viruses and clays in static and dynamic batch systems. Environmental Science & Technology. 2010; 44(12):4539-4544.
15. Yonggang Wang, Yusong LI, John D Fortner, Joseph B Hughes, Linda M Abriola, Kurt D Pennell. Transport and retention of nanoscale c60 aggregates in water-saturated porous media. Environmental Science & Technology. 2008; 42(10):3588-3594.
16. Tiantian Zhang, Michael Murphy, Haiyang Yu, Chun Huh, Steven L Bryant. Mechanistic model for nanoparticle retention in porous media. Transport in Porous Media. 2016; 115:387-406.
17. Tiantian Zhang, Michael J Murphy, Haiyang YU, Hitesh G Bagaria, Ki Youl Yoon, Bethany M Neilson, *et al*. Investigation of nanoparticle adsorption during transport in porous media. SPE Journal. 2015; 20(4):667-677.