



# The Kinetics of Reactions in the Mechanism of Ultraviolet Degradation of $H_2S$ Combined with the Non-Appearance of $O_2$ Using the Homotopy Perturbation Method

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**Received Date:** May 16, 2025

**Published Date:** June 09, 2025

## Abstract

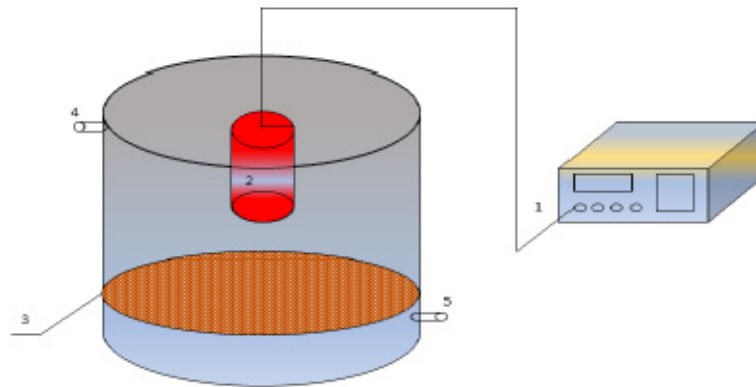
The presence of hydrogen sulphide has hampered the development of biogas energy. Traditional hydrogen sulphide photodegradation occurs in the presence of oxygen. However, this is inappropriate for biogas desulfurization and should be avoided. As a result, the current study is the first to investigate the theoretical UV degradation of  $H_2S$  in the absence of oxygen. First, a theoretical model of  $H_2S$  photodegradation was developed using the homotopy perturbation method, which included models of gas flow distribution and photoreactor radiation kinetics, mass balance, and degradation rate calculation. The impact of parameters such as  $H_2S$  mass and gas retention duration on the photodegradation rate was then investigated to validate the mathematical model. Furthermore, the rate of  $H_2S$  photodegradation increased as the retention time increased. The analytical results matched the experimental results extremely well, indicating that the mathematical model can be used to simulate  $H_2S$  photodegradation.

**Keywords:** Mathematical modelling;  $H_2S$  photodegradation; renewable energy techniques; nonlinear equations; and the homotopy perturbation method

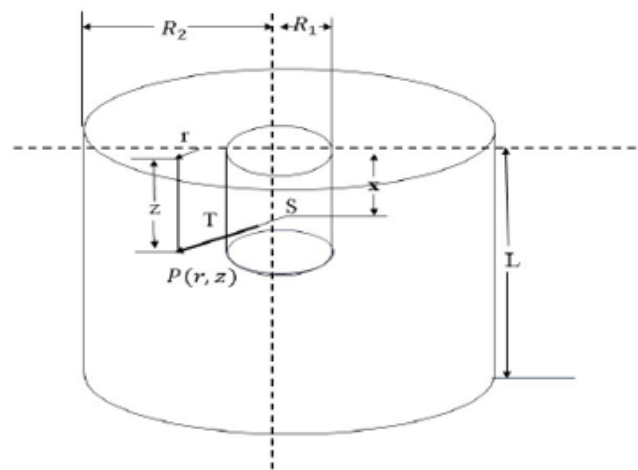
## Introduction

Anaerobic digestion, which is regarded as the most important strategy for producing renewable energy from biomass to recover clean biogas fuel, see [1], produces hydrogen sulphide [ $H_2S$ ], which contains 0.3%–0.4% of the material  $CH_4$  and  $CO_2$ , see [2].  $H_2S$  is a foul acid gas with the potential to cause significant corrosion in equipment, instruments, and pipelines. Furthermore,  $H_2S$  has a negative impact on people's health and the environment. When the biogas is used for energy (burning, generating power, etc.), the  $H_2S$  in it is converted to  $SO_2$ , which may significantly worsen air pollution (see [3]). Thus, the presence of  $H_2S$  impedes the promotion of biogas energy, and  $H_2S$  must be extracted from biogas using effi-

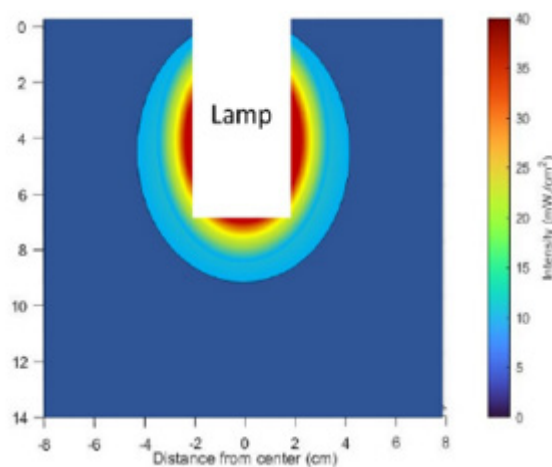
cient methods.  $H_2S$  techniques include biological, chemical, physical, and combinatorial technologies. The direct decomposition of  $H_2S$  to produce sulphur and hydrogen is a research topic for both domestic and international researchers because it allows for the recycling of hydrogen energy while also efficiently managing the  $H_2S$  pollution generated during the processing of coal, oil, gas, and minerals. Thermal [4,5], electrochemical [6], photocatalytic [7-9], and plasma degradation [10,11] are the primary  $H_2S$  degradation processes that produce hydrogen and sulphur. Photocatalytic  $H_2S$  degradation is the most promising technique available today due to its high treatment efficacy and reaction movement [12] (Figure 1-3).



**Figure 1:** H<sub>2</sub>S photodegradation reactor: 1. Generator with High Frequency, 2. Distribution of Gas Equipment 3. Electrodeless VUV Lamp, 4. Gas Outlet, 5. Gas Inlet.



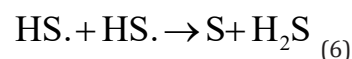
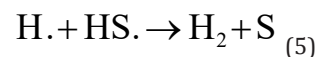
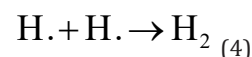
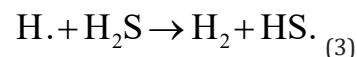
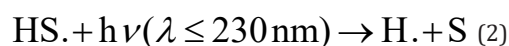
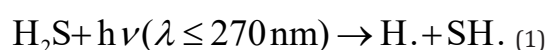
**Figure 2:** Cylindrical light source and Cylindrical photoreactor.



**Figure 3:** The distribution of light intensity within the photoreactor.

## Mathematical Formulation of the Problem

Wilson et al. [13] investigated the direct photodegradation of hydrogen sulphide ( $H_2S$ ) in the approaching Ultraviolet (UV) band. Photons with wavelengths below 270 nm can initiate degradation of  $H_2S$ , resulting in the formation of hydroxyl radicals ( $H\cdot$ ) and sulfhydryl radicals ( $SH\cdot$ ). Moreover, further photon exposure, particularly with wavelengths less than 230 nm, facilitated the transformation of  $SH\cdot$  into  $H\cdot$  and sulphur radicals ( $S\cdot$ ), as confirmed by experimental evidence (1), and (2). These reactions demonstrate the complex interplay between  $H_2S$  and UV radiation, focusing on the formation of reactive intermediates such as radicals and their subsequent reactions with oxygen and other environmental species. Further research into these reaction pathways is critical for understanding the fate and impact of  $H_2S$  photodegradation in various environmental settings.



The degradation rate equation for each intermediate during the photodegradation of hydrogen sulphide in the absence of oxygen can be determined using the relevant literature, the Technology's chemical dynamics database, and the National Institute of Standards based on (1), (2), (3), (4), (5), and (6), respectively. As a photon is presented in (1) and (2), the rate constants are denoted by  $k_{obs1}$ ,  $k_{obs2}$ ,  $k_3$ ,  $k_4$ ,  $k_5$ , and  $k_6$ . The reaction rates of each component can be expressed using the equations below:

$$\frac{d[H_2S]}{dt} = -k_{obs1}[H_2S] - k_3[H_2S][H\cdot] + k_6[SH\cdot] \quad (7)$$

$$\frac{d[H\cdot]}{dt} = k_{obs1}[H_2S] + k_{obs2}[SH\cdot] - k_3[H_2S][H\cdot] + k_4[H\cdot]^2 - k_5[SH\cdot][H\cdot] \quad (8)$$

$$\frac{d[SH\cdot]}{dt} = k_{obs1}[H_2S] + k_{obs2}[SH\cdot] - k_5[SH\cdot][H\cdot] - k_6[SH\cdot]^2 \quad (9)$$

$$\frac{d[H_2]}{dt} = k_3[H_2S][H\cdot] + k_4[H\cdot]^2 + k_5[H\cdot][SH\cdot] \quad (10)$$

$$\frac{d[S]}{dt} = k_{obs2}[SH\cdot] - k_5[SH\cdot][H\cdot] - k_6[SH\cdot]^2 \quad (11)$$

The initial conditions are given below:

$$\begin{aligned} t = 0, H_2S &= H_{2S_{ini}} \\ t = 0, H\cdot &= H_{\cdot_{ini}} \\ t = 0, SH\cdot &= SH_{\cdot_{ini}} \\ t = 0, H_2 &= H_{2_{ini}} \\ t = 0, S &= S_{ini} \end{aligned} \quad (12)$$

and the boundary conditions are

$$\begin{aligned} t = 0, H_2S &= 0 \\ t = 0, H\cdot &= 0 \\ t = 0, SH\cdot &= 0 \\ t = 0, H_2 &= 0 \\ t = 0, S &= 0 \end{aligned} \quad (13)$$

## Approximate Analytical Representation for the Concentration of H<sub>2</sub>S Photodegradation and the Corresponding Reaction Rate Equations for H<sub>2</sub>S, H, SH, H<sub>2</sub>, And S Using HPM

Many researchers in engineering and physics have recently used the Homotopy perturbation method to solve a wide range of nonlinear problems [14-19]. This method combines a conventional perturbation scheme with topology. J. H. He, used the Homotopy

perturbation method to solve the light hill equations [20], Duffing equations [21], and Blasius equations [22]. This method is notable for its efficiency, precision, and applicability. The Homotopy perturbation method uses the surrounding parameter  $p$  as a small parameter, and (Appendix A) it only takes a few duplications to find an asymptotic result. Using HPM (Appendix B), analytical expressions for the concentrations of H<sub>2</sub>S, H, SH, H<sub>2</sub>, and S are obtained using the homotopy perturbation method from these equations, giving the following results:

(Calculation was provided in the Supplementary Materials)

$$[H_2S]t = c_1 e_1^{-at} + \frac{1}{c_4} \left[ (L_1 - L_4 t) e_1^{-at} - L_2 e_1^{-at-bt} + L_3 e_1^{-2at} + c_{18} e_1^{-2bt} \right] \quad (14)$$

$$[H.]t = c_3 e_1^{-at} + e_1^{-bt} - c_2 + \frac{a}{c_4} \left[ L_1 \frac{e_1^{-at}}{-a} - L_4 \left( t \frac{e_1^{-at}}{-a} - \frac{e_1^{-at}}{a^2} \right) - L_2 \frac{e_1^{-(a+b)t}}{-(a+b)} + L_3 \frac{e_1^{-2at}}{-2a} + c_{18} \frac{e_1^{-2bt}}{-2b} \right] + \frac{b}{p_{98}} \left[ A_1 \frac{e_1^{-2bt}}{-2b} - A_2 \frac{e_1^{-bt}}{b} + (p_{43} - p_{71} + p_{91}) \left( t \frac{e_1^{-bt}}{-b} - \frac{e_1^{-bt}}{b^2} \right) + (A_3 + A_6) \frac{e_1^{-(a+b)t}}{-(a+b)} - A_4 \frac{e_1^{-at}}{-a} + (p_{16} - p_{44} + p_{72}) \left( t \frac{e_1^{-at}}{-a} - \frac{e_1^{-at}}{a^2} \right) \right] - k_3 c_1 c_3 \frac{e_1^{-2at}}{-2a} + c_1 k_3 \frac{e_1^{-(a+b)t}}{-(a+b)} - c_1 c_2 k_3 \frac{e_1^{-at}}{-a} + k_4 \left[ c_3^2 \frac{e_1^{-2at}}{-2a} - 2c_3 \frac{e_1^{-(a+b)t}}{-(a+b)} + 2c_2 c_3 \frac{e_1^{-at}}{-a} + 2c_2 \frac{e_1^{-bt}}{b} - \frac{e_1^{-2bt}}{2b} + c_2^2 t \right] + k_5 \left[ A \frac{e_1^{-(a+b)t}}{(a+b)} + A c_3 \frac{e_1^{-2at}}{2a} - A c_2 \frac{e_1^{-at}}{-a} + B c_3 \frac{e_1^{-(a+b)t}}{(a+b)} - B c_2 \frac{e_1^{-bt}}{b} + B \frac{e_1^{-2bt}}{2b} \right] \quad (15)$$

$$[SH.]t = A e_1^{-at} + B e_1^{-bt} + \frac{e_1^{-3at-2bt}}{p_{98}} \left[ A_1 e_1^{3at} + e_1^{3at+bt} (A_2 + p_{43}t - p_{71}t + p_{91}t) + (A_3 + A_6) e_1^{(2a+b)t} + e_1^{(2a+2b)t} (A_4 + p_{16}t - p_{44}t + p_{72}t) + A_5 e_1^{(a+2b)t} \right] \quad (16)$$

$$[H_2]t = H_{2ini} + k_3 c_1 c_3 \frac{e_1^{-2at}}{2a} + c_1 k_3 \frac{e_1^{-(a+b)t}}{-(a+b)} - c_1 c_2 k_3 \frac{e_1^{-at}}{-a} + k_4 \left[ c_3^2 \frac{e_1^{-2at}}{-2a} - 2c_3 \frac{e_1^{-(a+b)t}}{-(a+b)} + 2c_2 c_3 \frac{e_1^{-at}}{-a} + 2c_2 \frac{e_1^{-bt}}{b} - \frac{e_1^{-2bt}}{2b} + c_2^2 t \right] + k_5 \left[ A \frac{e_1^{-(a+b)t}}{(a+b)} + A c_3 \frac{e_1^{-2at}}{2a} - A c_2 \frac{e_1^{-at}}{-a} + B c_3 \frac{e_1^{-(a+b)t}}{(a+b)} - B c_2 \frac{e_1^{-bt}}{b} + B \frac{e_1^{-2bt}}{2b} \right] \quad (17)$$

$$\begin{aligned}
[S]t = & b \left[ A \frac{e_1^{-at}}{-a} + B \frac{e_1^{-bt}}{-b} \right] + S_{ini} + b \left[ \frac{A}{a} + \frac{B}{b} \right] \\
& + \frac{b}{p_{98}} \left[ A_1 \frac{e_1^{-2bt}}{-2b} - A_2 \frac{e_1^{-bt}}{b} + (p_{43} - p_{71} + p_{91}) \left( t \frac{e_1^{-bt}}{-b} - \frac{e_1^{-bt}}{b^2} \right) \right. \\
& \left. + (A_3 + A_6) \frac{e_1^{-(a+b)t}}{-(a+b)} - A_4 \frac{e_1^{-at}}{-a} + (p_{16} - p_{44} + p_{72}) \left( t \frac{e_1^{-at}}{-a} - \frac{e_1^{-at}}{a^2} \right) \right] \\
& + k_5 \left[ Ac_3 \frac{e_1^{-2at}}{2a} + Bc_3 \frac{e_1^{-(a+b)t}}{(a+b)} + A \frac{e_1^{-(a+b)t}}{(a+b)} + B \frac{e_1^{-2bt}}{2b} - Ac_2 \frac{e_1^{-at}}{a} - Bc_2 \frac{e_1^{-bt}}{b} \right] \\
& + k_6 \left[ A^2 \frac{e_1^{-2at}}{-2a} - 2AB \frac{e_1^{-(a+b)t}}{(a+b)} - B^2 \frac{e_1^{-2bt}}{2b} \right] \quad (18)
\end{aligned}$$

## Results and their discussions

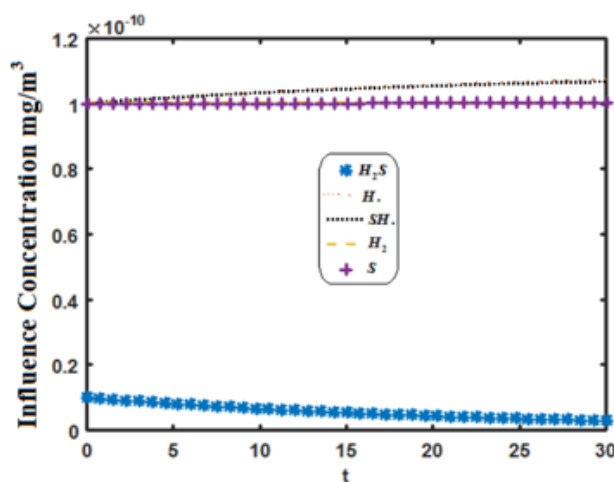
### Proposed Model of H<sub>2</sub>S Photodegradation

The cylindrical VUV lamp is placed in the centre of the photo-reactor's virtualized three-dimensional representation of light intensity, with a diameter of 15 cm and a height of 14 cm, as shown in (Figure 3). The VUV lamp in the white region measures 4 cm in diameter and 5.8 cm in height, as depicted in the illustration. Figure 3 shows how the intensity of light rapidly decreases as one moves away from the light source's centre, see [12].

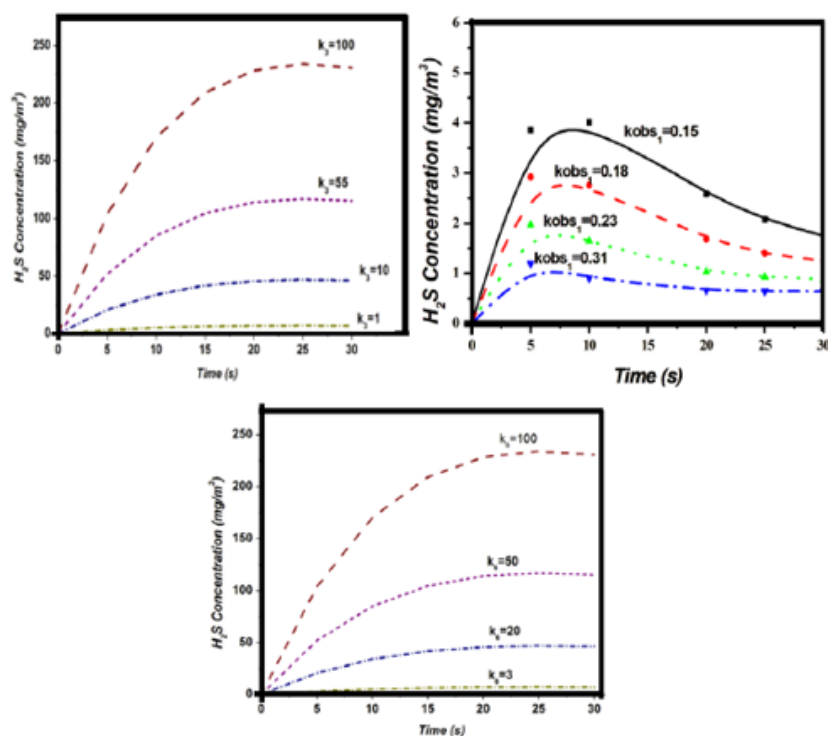
### Major Influence Factors on H<sub>2</sub>S Photodegradation

Equations (14)-(18) represent the approximate analytical expressions for the concentrations of H<sub>2</sub>S, H., SH., H<sub>2</sub>, and S. Figure 3 depicts the concentration evolution of H<sub>2</sub>S, H., SH., H<sub>2</sub>, and S calculated 2cm away from ultraviolet light and displayed by the analytical solution (14)-(18). Figure 4 depicts influence concentration

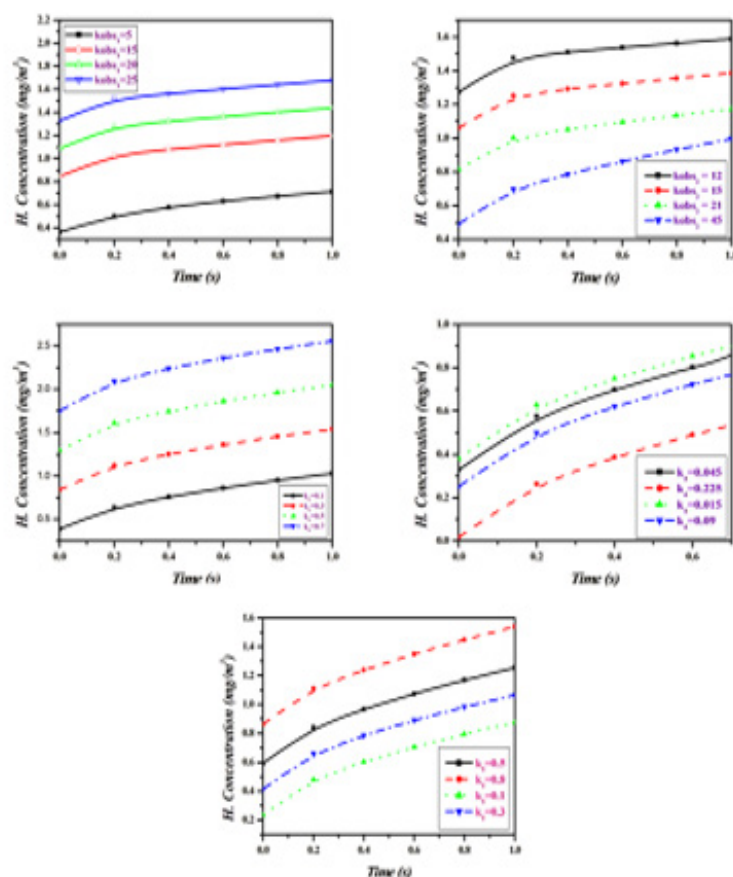
for various values (analytical) as compared to experimental results [12]. Figure 5 depicts the impact of initial gas retention and H<sub>2</sub>S concentration duration on photodegradation rate. Constant  $k_3$  and  $k_6$  increased, as did the concentration of H<sub>2</sub>S and  $k_{obs1}$  has decreased. Figure 6 shows that the simulated concentration of H. radicals increased, whereas  $k_{obs1}$ ,  $k_1$ , and  $k_5$  decreased.  $k_{obs2}$  and  $k_4$  have increased and H. concentration decreased. Figure 7 also shows that the concentration SH. increased,  $k_{obs1}$ ,  $k_5$  increased, and  $k_{obs2}$  and  $k_6$  decreased. Figure 8 depicts the accelerating rate of degradation. Figure 9 indicates that the simulated concentration S increased, decreased, and increased. Mathematical analysis of the simulated concentrations for the elements of H<sub>2</sub>S photodegradation by Ultra Violet in the absence of oxygen. The concentration changes of H<sub>2</sub>S, H., SH., H<sub>2</sub>, and S. The model incorporates a set of steady-state non-linear reaction-diffusion equations. Applying the homotopy perturbation scheme to these equations yields analytical expressions for concentrations.



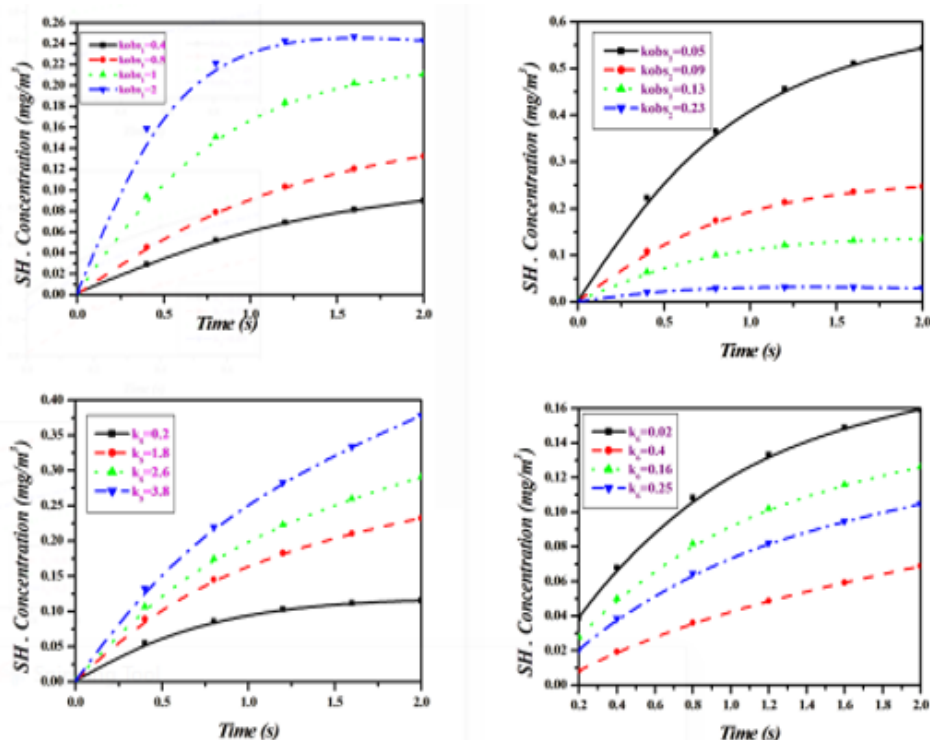
**Figure 4:** represents influence concentration for different values and compared experimental results.



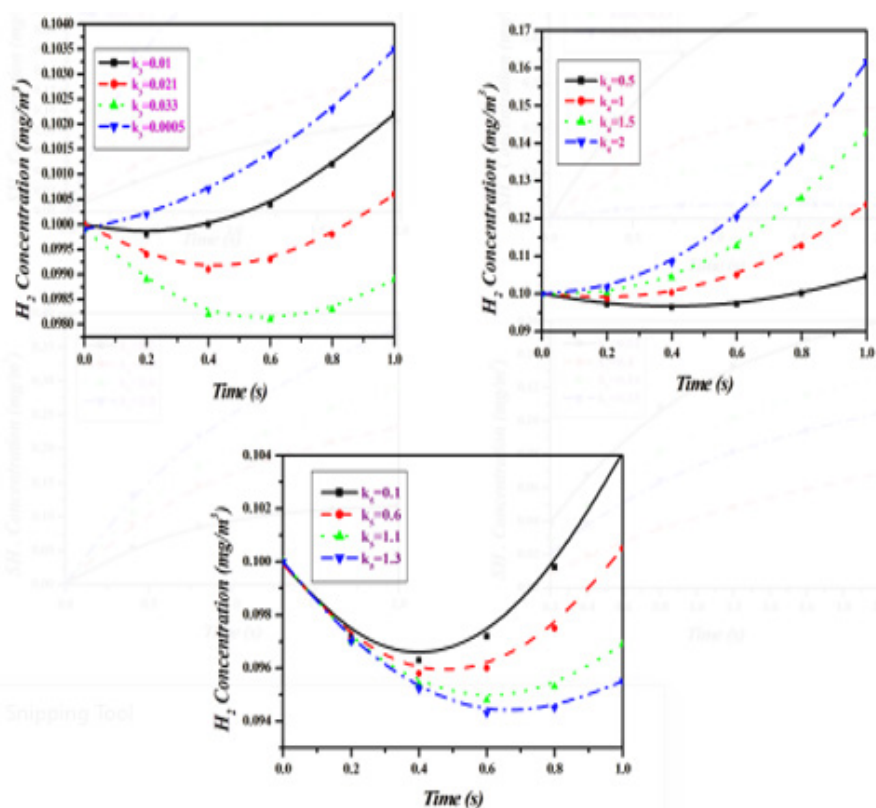
**Figure 5:** Plot of Influence Concentration profile versus time  $t$  computed with Equation (14) for different experimental parameter values  $k_{obs1}=0.15$ ,  $k_{obs2}=0.00014$ ,  $k_3=0.2 \times 10^2$ ,  $k_6=0.2 \times 10^2$ .



**Figure 6:** Plot of influence concentration profile versus time  $t$  computed with Equation (15) for different experimental parameter values  $k_{obs1}=5$ ,  $k_{obs2}=12$ ,  $k_3=0.1$ ,  $k_4=0.045$ ,  $k_5=0.5$ .

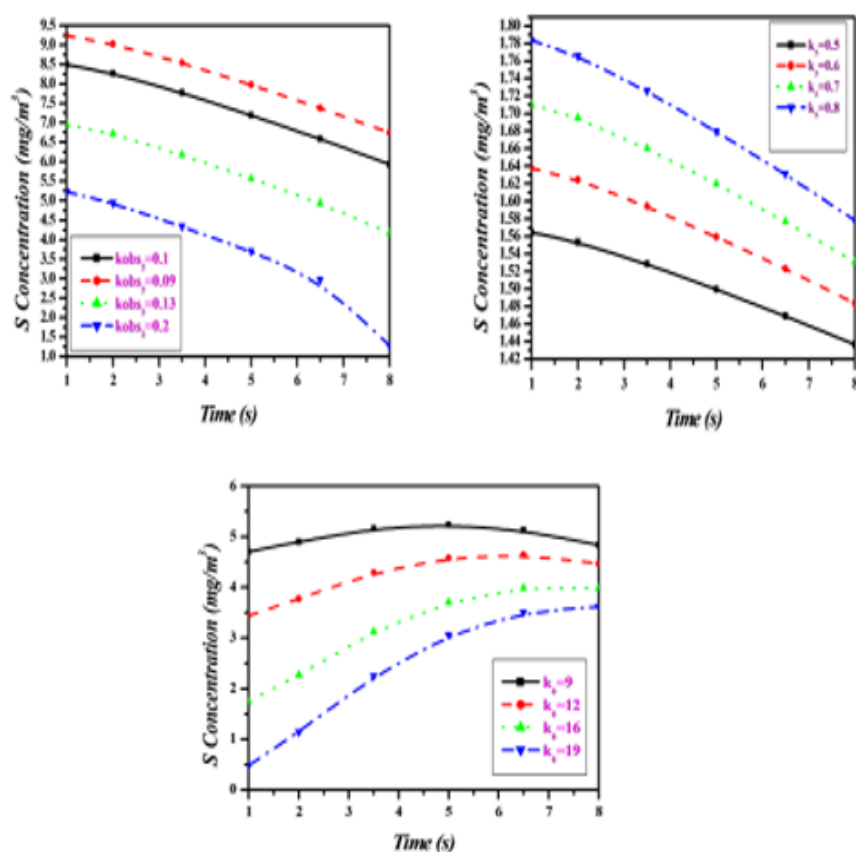


**Figure 7:** Plot of influence concentration profile versus time  $t$  computed with Equation (16) for different experimental parameter values  $k_{obs1}=0.4$ ,  $k_{obs2}=0.05$ ,  $k_5=0.2$ ,  $k_6=0.02$ .



**Figure 8:** Plot of influence concentration profile versus time  $t$  computed with Equation (17) for different experimental parameter values  $k_{obs1}=1$ ,  $k_{obs2}=0.1$ ,  $k_3=0.01$ ,  $k_4=0.5$ ,  $k_5=0.1$ .





**Figure 9:** Plot of influence concentration profile versus time  $t$  computed with Equation (18) for different experimental parameter values  $k_{obs1}=1$ ,  $k_{obs2}=0.1$ ,  $k_5=0.5$ ,  $k_6=9$ .

## Conclusion

In the article's overall conclusion and future development, the proposed model of UV degradation of  $H_2S$  was determined without the presence of oxygen, and the impact of the initial  $H_2S$  concentration and gas preservation duration on the photodegradation experiment was associated with the analytical results. In this work, the nonlinear differential equations in the VUV degradation are solved

analytically using HPM, and an approximate and closed analytical representation form of the concentration of  $H_2S$ ,  $H$ ,  $SH$ ,  $H_2$ , and  $S$  is provided. These novel analytical findings provide an intuitive understanding of the system and allow parameter optimization for VUV photodegradation of  $H_2S$  in the absence of oxygen.

## Conflict of interest

The authors declare no competing financial interest.

## Nomenclature

Symbols	Description	Units
$H_2S$	Influence Concentration	$mg/m^3$
$H$	Influence Concentration	$mg/m^3$
$SH$	Influence Concentration	$mg/m^3$
$H_2$	Influence Concentration	$mg/m^3$
$S$	Influence Concentration	$mg/m^3$
$k_{obs1}$	Rate Constants	$m^{-1}s^{-1}$



$k_{obs2}$	Rate Constants	$m^{-1}s^{-1}$
$k_3$	Rate Constants	$m^{-1}s^{-1}$
$k_4$	Rate Constants	$m^{-1}s^{-1}$
$k_5$	Rate Constants	$m^{-1}s^{-1}$
$k_6$	Rate Constants	$m^{-1}s^{-1}$

## Data Availability Statement

The data sets used and/or analysed during the current study are available from the corresponding author upon reasonable request.

## Author's Contributions

Methodology, Validation and Investigation: K. Saranya; Resource, Visualization and Writing-Original draft: M. Suguna; Visualization, Formal Analysis and Writing-review and editing: Salahuddin. All authors have read and agreed to the published version of the manuscript.

## Disclosure of Interest

No potential conflict of interest was reported by the authors.

## Funding

This research is supported by the Deanship of Graduate Studies and Scientific Research at Jazan University in Saudi Arabia, under Project number GSSRD-24.

## Acknowledgement

The authors gratefully acknowledge the funding of the Deanship of Graduate Studies and Scientific Research, Jazan University, Saudi Arabia, through Project Number: GSSRD-24.

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