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Mathematical Modeling and Optimal Control of Carbon Dioxide Emissions

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Abstract. This paper aims to demonstrate the flexibility of mathematical models in analyzing carbon dioxide emissions and account for memory effects. The use of real data amplifies the importance of this study. This research focuses on developing a mathematical model utilizing fractional-order differential equations to represent carbon dioxide emissions stemming from the energy sector. By comparing simulation results with real-world data, it is determined that the fractional model exhibits superior accuracy when contrasted with the classical model. Additionally, an optimal control strategy is proposed to minimize the levels of carbon dioxide, CO_2, and associated implementation costs. The fractional optimal control problem is addressed through the utilization of an iterative algorithm, and the effectiveness of the model is verified by presenting comparative results.

Keywords. Fractional, Mathematical model, Optimal control, Carbon dioxide.

MSC. 34A08; 65k10; 92B05.

1 Introduction

In recent decades, economic growth and associated increases in industrial production across the world have led to an increase in energy consumption, with burning fossil fuels supplying around 80% of the world's energy [6]. When fossil fuels are burned, they release large amounts of carbon dioxide, a greenhouse gas, into the air. The Intergovernmental Panel on Climate Change (IPCC) has found that emissions from fossil fuels are the dominant cause of global warming. In 2018, 89% of global CO_2 emissions came from fossil fuels and industry [9]. To decrease CO_2 emissions from the energy source, various methods can be used, including energy efficiency, the help of renewable energy, fuel switching, and the more efficient use and recycling of materials [12]. In recent years, mathematical modeling has become a valuable tool to study the effect of different factors on the dynamics of atmospheric carbon dioxide gas, and appraise strategies to control. In most cases, differential equations of the integer order have been used to construct such models. L. Han et al. introduced a carbon absorption-emission model with a delay in [8], which was based on carbon emission and absorption. In [7], a mathematical model was explored for carbon emissions and optimizing process parameters in laser welding cells. Several nonlinear dynamical models are proposed to derive the optimal strategies for mitigating carbon dioxide emission in [16, 17]. The integer-order derivatives and integrals have local properties, meaning that the next state is not influenced by the current and previous state. The integer-order mathematical models cannot describe natural phenomena precisely.

Fractional calculus is an extension of classical calculus which introduces derivatives and integrals of fractional order. Fractional derivatives have non-local properties, meaning that the next state depends on the current state and all previous states. This is the main excellence of fractional derivatives over classical derivatives. Fractional calculus is currently utilized as a significant means for studying dynamic systems. Baleanu et al. explored two generalized fractional models with a real case study in [4, 5]. In [10], a comparison analysis was made between different operators in fractional dynamical systems. Srivastava et al. analyzed a biological population model with carrying capacity using fractional-order calculations in [14]. In [13], a computational analysis of a fractional model for the dynamics of carbon dioxide gas in the atmosphere was conducted.

For further research, refer to [2, 3, 15], and the accompanying references.

In light of this notable advantage, we were motivated to extend the model studied in [17] to a novel fractional model involving the Caputo derivatives. We aim to demonstrate that fractional mathematical models have greater flexibility to analyze carbon dioxide emissions and account for memory effects. The use of real data adds importance to this study. To the best of our knowelege, this is the first work that employs a non-local derivative operator in modeling the CO_2 emissions from the energy sector and its optimal control treatment.

2 Fractional Model

In this section, we propose a fractional mathematical model for the carbon dioxide emissions from the energy sector. The original version of this model is a system of nonlinear ordinary differential equations as presented in [17]. However, this model does not consider the effect of previous states in the current states of CO_2 emissions. One way to overcome this drawback is to replace the integer-order derivatives in the model with non-integer-order derivatives. Therefore, we replace the ordinary derivative with the Caputo fractional derivative operator. Thus, the new model is described by the following system:

$$\begin{cases} {}_{0}^{c}D_t^{\nu}C(t) = -\alpha\left(C - C_0\right) + \mu_1 N + \mu_2\left(1 - \eta_2\right)E, \\ {}_{0}^{c}D_t^{\nu}N\left(t\right) = rN\left(1 - \frac{N}{L}\right) + \kappa_1 NE + \kappa_2 N^2 E - \theta\left(C - C_0\right)N, \\ {}_{0}^{c}D_t^{\nu}E\left(t\right) = \left(1 - \eta_1\right)\frac{\gamma \mathrm{NE}}{K+N} - \gamma_0 E^2, \\ C\left(0\right) \geq C_0,\ N\left(0\right) \geq 0,\ E\left(0\right) \geq 0, \end{cases} \tag{1}$$

where ${}_{0}^{c}D_t^{\nu}$ is the Caputo fractional derivative of order $0 < \nu \leq 1$ and is defined for an arbitrary function $\Phi(t)$ as follows [11]:

$$ {}_{0}^{c}D_t^{\nu}\Phi(t) = \frac{1}{\Gamma(1-\nu)}\int_0^t (t-\tau)^{-\nu}\Phi^{'}(\tau)d\tau. $$

Moreover, when $\nu = 1$, the model becomes an integer model. In this model, $C(t), N(t)$, and $E(t)$ represent atmospheric CO_2 concentration, human population, and energy use at time t, respectively. All parameters in the model are non-negative. The descriptions of the parameters given as follow:

- C_0 denotes pre-industrial CO_2 concentration, α is the removal rate of atmospheric CO_2 by the sinks of CO_2.
- μ_1 represents the emission rate coefficients of CO_2 from non-energy sectors, μ_2 is the emission rate coefficients of CO_2 from energy sectors.
- η_2 denotes the efficiency of mitigation options to curtail the CO_2 emission rate per unit of energy use.
- r denotes the intrinsic growth rate, L is the carrying capacity of the population.
- κ_1 is the growth rate coefficients of population, κ_2 is carrying capacity of population due to energy use.
- θ is the mortality rate coefficient of the population due to the adverse impacts posed by enhanced CO_2 levels.
- γ denotes the growth rate of energy use, γ_0 is the depletion rate of energy use, K is half-saturation constant. η_1 denotes the efficiency of mitigation options to cut down the energy consumption rate through increasing energy efficiency and bringing the behavioral changes in people.

3 Optimal Control

Reducing atmospheric CO_2 levels can be achieved by decreasing the rate at which it is produced during energy generation and limiting the increase in energy consumption. The most effective methods for lowering CO_2 levels have minimal costs for mitigation. Optimal control theory can be used to develop these strategies and minimize implementation costs. In this section, we use optimal controllers based on Pontryagin's Minimum Principle (PMP) to stabilize the behavior of the fractional-order system described by (1). To achieve this, we assume that the parameters η_1 and η_2 are Lebesgue measurable functions of time on the interval $[0, t_f]$. Therefore, model (1) is rewritten as follows:

$$\begin{cases} {}_{0}^{c}D_t^{\nu}C(t) = -\alpha\left(C - C_0\right) + \mu_1 N + \mu_2\left(1 - \eta_2(t)\right)E, \\ {}_{0}^{c}D_t^{\nu}N\left(t\right) = rN\left(1 - \frac{N}{L}\right) + \kappa_1 NE + \kappa_2 N^2 E - \theta\left(C - C_0\right)N, \\ {}_{0}^{c}D_t^{\nu}E\left(t\right) = \left(1 - \eta_1(t)\right)\frac{\gamma \mathrm{NE}}{K+N} - \gamma_0 E^2, \\ C\left(0\right) \geq C_0,\ N\left(0\right) \geq 0,\ E\left(0\right) \geq 0 \end{cases} \tag{2}$$

We consider the state system (2) of fractional differential equations, where the set of admissible control functions are given by

$$\Omega = \{(\eta_1(t), \eta_2(t)) \in (L^\infty(0, t_f))^2 : 0 \leq \eta_1(t) \leq \eta_{1\,\max}, 0 \leq \eta_2(t) \leq \eta_{2\,\max}\}.$$

The objective is to minimize both the level of CO_2 and the cost of implementing mitigation options by minimizing the following objective functional:

$$I = \int_0^{t_f} (w_1 C(t) + w_2 \eta_1^2(t) + w_3 \eta_2^2(t))dt, \tag{3}$$

where the constants w_1, w_2 and w_3 are weighting coefficients.

We consider the optimal control problem of finding $(C^*(\cdot), N^*(\cdot), E^*(\cdot))$ associated with an admissible control pair $(\eta_1^*(\cdot), \eta_2^*(\cdot)) \in \Omega$ on the time interval $[0, t_f]$, which satisfies (2) and minimizes the cost functional (3). To address this problem, we use a kind of the PMP in the fractional order state as proposed in [1]. We define the Hamiltonian function as below:

$$\begin{aligned} H = {} & w_1 C(t) + w_2 \eta_1^2(t) + w_3 \eta_2^2(t) \\ & + \rho_1(t)\big(-\alpha(C - C_0) + \mu_1 N + \mu_2(1 - \eta_2(t))E\big) \\ & + \rho_2(t)\big(rN(1 - \frac{N}{L}) + \kappa_1 NE + \kappa_2 N^2 E - \theta(C - C_0)N\big) \\ & + \rho_3(t)\big((1 - \eta_1(t))\frac{\gamma NE}{K + N} - \gamma_0 E^2\big), \end{aligned}$$

where $\rho_i(t)$ $(i = 1, 2, 3)$ are the co-state variables. The optimality conditions are obtained from the following conditions:

$$\frac{\partial H}{\partial \eta_1} = 0, \quad \frac{\partial H}{\partial \eta_2} = 0.$$

Hence, we have

$$\eta_1 = \frac{\rho_3}{2w_2}\frac{\gamma NE}{K + N}, \quad \eta_2 = \frac{\rho_1}{2w_3}\mu_2 E, \tag{4}$$

on interior of set Ω, where the adjoint variables satisfy

$$\begin{aligned} {}_0^cD_t^\nu \rho_1(t) &= -\frac{\partial H}{\partial C} = -w_1 + \rho_1\alpha + \theta\rho_2 N, \\ {}_0^cD_t^\nu \rho_2(t) &= -\frac{\partial H}{\partial N} \\ &= -\rho_1\mu_1 - \rho_2\big(r(1 - \frac{2N}{L}) + \kappa_1 E + 2\kappa_2 NE - \theta(C - C_0)\big) - \frac{\rho_3(1 - \eta_1)\gamma KE}{(K + N)^2}, \\ {}_0^cD_t^\nu \rho_3(t) &= -\frac{\partial H}{\partial E} = -\rho_1\mu_2(1 - \eta_2) - \rho_2(\kappa_1 N + 2\kappa_2 N^2) - \rho_3\big((1 - \eta_1)\frac{\gamma N}{K + N} - 2\gamma_0 E\big), \\ \rho_1(t_f) &= \rho_2(t_f) = \rho_3(t_f) = 0. \end{aligned}$$

Then, we have the following boundary value problem for optimal treatment:

$$\begin{cases} {}_0^cD_t^\nu C(t) = -\alpha\left(C - C_0\right) + \mu_1 N + \mu_2\left(1 - \eta_2\right)E, \\ {}_0^cD_t^\nu N\left(t\right) = rN\left(1 - \frac{N}{L}\right) + \kappa_1 NE + \kappa_2 N^2 E - \theta\left(C - C_0\right)N, \\ {}_0^cD_t^\nu E\left(t\right) = \left(1 - \eta_1\right)\frac{\gamma \mathrm{NE}}{K+N} - \gamma_0 E^2, \\ {}_0^cD_t^\nu \rho_1(t) = -\frac{\partial H}{\partial C} = -w_1 + \rho_1\alpha + \theta\rho_2 N, \\ {}_0^cD_t^\nu \rho_2(t) = -\frac{\partial H}{\partial N} = -\rho_1\mu_1 - \rho_2\big(r(1 - \frac{2N}{L}) + \kappa_1 E + 2\kappa_2 NE \\ -\theta(C - C_0)\big) - \dfrac{\rho_3(1 - \eta_1)\gamma KE}{(K + N)^2}, \\ {}_0^cD_t^\nu \rho_3(t) = -\frac{\partial H}{\partial E} = -\rho_1\mu_2(1 - \eta_2) - \rho_2(\kappa_1 N + 2\kappa_2 N^2) \\ -\rho_3\big((1 - \eta_1)\frac{\gamma N}{K+N} - 2\gamma_0 E\big), \\ \rho_1(t_f) = \rho_2(t_f) = \rho_3(t_f) = 0, \\ C\left(0\right) \geq C_0,\ N\left(0\right) \geq 0,\ E\left(0\right) \geq 0, \end{cases} \tag{5}$$

where $\eta_1(t)$ and $\eta_2(t)$ are given by (4). In turn, the optimality conditions PMP establish that the optimal controls $\eta_1(t)$ and $\eta_2(t)$ are defined by:

$$\eta_1^*(t) = \max\{min(\frac{\rho_3}{2w_2}\frac{\gamma NE}{K+N}, \eta_{1\,\max}), 0\},$$
$$\eta_2^*(t) = \max\{min(\frac{\rho_1}{2w_3}\mu_2 E, \eta_{2\,\max}), 0\}.$$

4 Simulation Results and Discussion

In this section, the effects of fractional operators on the behavior of the controlled system for the relationship between the human population, energy use, and atmospheric carbon dioxide are investigated. To do so, we apply the numerical algorithm expressed in the following to solve the coupled system (5).

4.1 Numerical algorithm

In this part, we develop the fractional version of fourth order Runge- Kutta (RK4) algorithm for the coupled system (5), as follows:

Algorithm 11

- Step1. Set the initial values for the control functions $\eta_1^*(t)$ and $\eta_2^*(t)$.
- Step2. Use the current values of control functions and apply the forward fractional RK4 method for the control system and obtain the original variables.
- Step3. Apply the backward fractional RK4 method to compute the adjoint variables using the current values of the original variables and control functions.
- Step4. Update the value of control functions.
- Step5. If the updated values of the original variables, adjoint variables and control functions are not close enough to their previous values, go to Step 2.

4.2 Simulation results

The simulation results in this study are based on the real data of atmospheric CO_2 concentration and global energy use are selected based on NOAA and World in Data for the period 1960 to 2021. Therefore, the real data of the year 1960 is set as the initial conditions:

$$C(0) = 316, N(0) = 3.032, \text{ and } E(0) = 40.5889.$$

The estimated values of the model parameters are as follows:

$$\alpha = 0.01621, C_0 = 280, \mu_1 = 0.1025, \mu_2 = 0.02698, r = 0.0265, L = 11,$$

$$\kappa_1 = 1.178 \times 10^{-5}, \kappa_2 = 1.2 \times 10^{-6}, \theta = 2.2183 \times 10^{-7}, \gamma = 0.08595,$$

$$K = 3.2, \gamma_0 = 0.0002575, \eta_1 = 0.1, \eta_2 = 0.1, \eta_{1\,\max} = 0.3, \eta_{2\,\max} = 0.5,$$

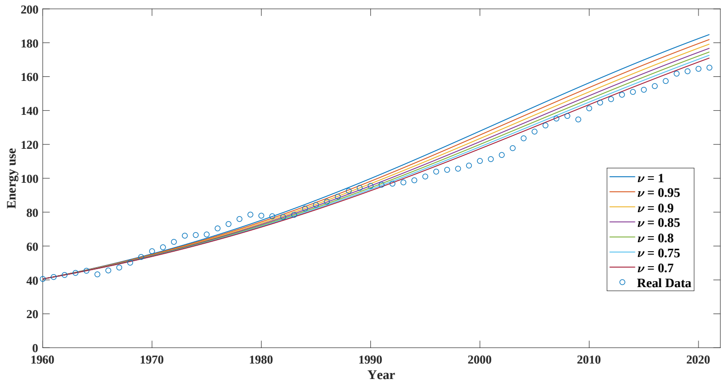

Figure 1: Comparison between the numerical solutions of carbon dioxide, and energy use based on the classic and fractional order models with real data.

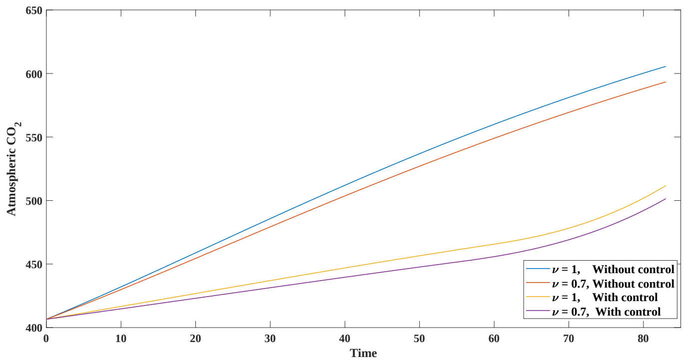

Figure 2: Numerical solutions of atmospheric CO2, with uncontrolled and controlled conditions for classic and fractional order models.

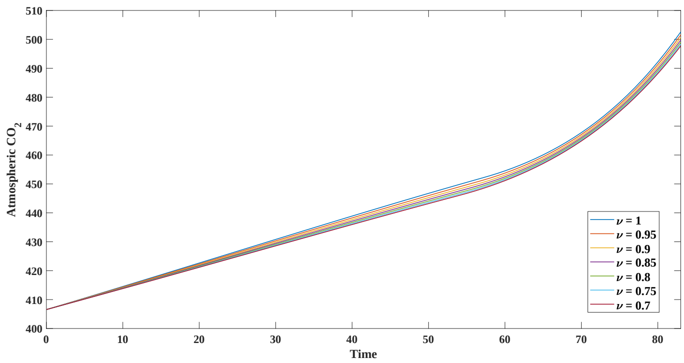

Figure 3: Numerical solutions of atmospheric CO2, fractional model with mitigation strategies for the control of future CO2 for various fractional order values.

and

$$w_1 = 1, w_2 = 100, w_3 = 100.$$

To demonstrate the efficiency of the new fractional model, the numerical results of carbon dioxide concentration and global energy use have been compared with the real data in Figure 1. In this figure, the diagrams of carbon dioxide concentration and energy use are plotted for the different values of the fractional order and the classic integer-order, and they are compared with the real data. This validation shows that the accuracy of new fractional system is better than the classic system. Moreover, with the increase of time, decreasing the fractional derivative order leads to more efficient numerical solutions, which converge towards the real data. Additionally, the difference between the accuracy of the fractional model and the classic model is more significant with the passage of time.

In this study, we will examine the efficiency of mitigation optimal control strategy on future CO_2 levels. To achieve this, we compare the atmospheric CO_2 concentration for controlled and uncontrolled conditions for the values of $\nu = 0.7$ and $\nu = 1$, in Figure 2. The initial conditions are based on the year 2017 set to $C(0) = 406.55, E(0) = 153.5956$ and $N(0) = 7.511$. The results show that applying the control strategy results leads in a significant reduction of atmospheric CO_2 concentration. In addition, the effect of this control scheme on the fractional system is more successful than the classical system. Furthermore, the future CO_2 level on the fractional model is investigated in Figure 3 for various fractional order values. As can be seen in this figure, the efficiency of the controls increases by moving away from the integer-order and reducing the fractional orders. In addition, the concentration of CO_2 grows up with the increase of fractional orders and tends uniformly to the integer-order trajectory.

5 Conclusion

This paper introduces a fractional mathematical model for carbon dioxide emissions and investigates the stability of the fractional-order system using optimal controllers based on Pontryagin's Minimum Principle. The fractional optimal control problem is solved using a forward-backward sweep iterative algorithm. Simulation results indicate that the fractional model provides a better approximation compared to the classic integer-order model.

Declarations

Availability of supporting data

All data generated or analyzed during this study are included in this published paper.

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Competing interests

The authors have no competing interests to declare that are relevant to the content of this paper.

Authors' contributions

The main manuscript text is written collectively by the authors.

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