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## Fractional order reaction-diffusion dynamics: A study via approximate analytical technique

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### Abstract

Lyons and colleagues proposed a model based on a second-order nonlinear differential equation to theoretically examine the steady-state of amperometric  $z$  behavior in polymer-modified electrode systems controlled by Michaelis-Menten (MM) kinetics. This study builds on previous work by extending the model to a Fractional Differential Equation (FDE) framework in order to better represent sequential dynamics. The impacts of different factors across multiple fractional orders  $\mu$  are analyzed in order to derive approximated analytical solutions for the FDE system using the Homotopy Perturbation Method (HPM). The fractional-order technique allows for a smooth transition between fractional and integer-order dynamics and enables more flexibility for simulating complex reaction-diffusion phenomena. These findings contribute to a deeper understanding of the interaction between reaction kinetics and diffusion processes, opening new possibilities for advanced applications in electrochemical systems.

**Keywords:** Electro active polymer film, second-order ordinary differential equation, caputo fractional derivative, homotopy perturbation method

### Introduction

Electrode surfaces covered with electro active polymers films have become more popular in the domains of electro catalysis, chemical sensor technology, and energy storage applications. The development of polymer-based materials for electro catalysis and sensors, particularly those intended to function in batch amperometric  $z$  mode, has advanced significantly during the last ten years. A theoretical model for measuring the operational  $z$  properties of metal Oxide-Nafion composite amperometric sensors is presented in [3]. By describing their kinetics using the Michaelis-Menten formalism, these sensors' heterogeneous redox catalytic process provides insight into the interactions between substrates and sensor elements. Reference [6] provides a theoretical analysis of the steady-state  $z$  amperometric response in systems with polymer-modified electrodes. This investigation most likely looks into how other elements affecting sensor performance interact with substrate diffusion within the polymer matrix. Together, these studies advance our understanding of how substrates interact with sensor elements, whether through redox catalysis or substrate diffusion within polymer matrices. Ultimately, they contribute to the development of more efficient and sensitive sensors for a wide range of analytical and energy-related applications.

Fractional Calculus is an extension of the classical calculus of integer order. Fractional differential equations (FDEs) a cumulative advantage over integer-order differential equations (IDEs) in modeling complex real-world issues due to their unique features. Because of their memory effects, FDEs are more efficient than IDEs, which are by nature local. The application of fractional derivatives in various scientific and technical fields has led to their significant advancement in recent years. When modeling real-life events, FDEs are a useful tool for minimizing errors caused by overlooked parameters. See [14] noted in their investigation of electrochemistry and fractional calculus to improve our understanding of how chemical reactions at electrodes affect electric currents and concentration dynamics in electrochemical systems. In [26], integrates mathematical modeling with biochemical processes to clarify the dynamics of enzyme inhibitor reactions, demonstrating the effectiveness of fractional calculus in handling the complexities of biological systems. Reference [24] discusses sequential and non-sequential Caputo fractional differential equations, their definitions, solution existence, and numerical methods. It emphasizes the advantages of sequential equations in real-world applications and suggests future research directions in fractional calculus.

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The numerical solution of sequential case can also be determined, potentially producing solutions that converge to integer boundary value problems. See [27], provided the idea of fractional differentiation and integration with their basic properties. The semi-analytical HPM provides multiple advantages for addressing nonlinear case. It is straightforward and efficient, yielding analytical or semi-analytical solutions without requiring small perturbation parameters. HPM is versatile, applicable to various problems across disciplines like engineering and physics, and excels in handling strong nonlinearities and complex boundary conditions. The Fractional Homotopy Perturbation Method (FHPM) is an extension of the HPM designed to solve fractional derivatives, which involve derivatives of non-integer order. FHPM effectively captures the memory and hereditary properties of complex systems, and demonstrating good convergence and computational efficiency. The basic concept of FHPM for an FDE system has been explained in [27].

This paper discusses a mathematical model developed by Lyons and colleagues [6], which focuses on the formation of a substrate for complex with a immobilized catalyst complex on a surface. Initially, this model is formulated as a second-order nonlinear differential equation with boundary conditions. We modified it to a  $z$  Caputo-fractional differential equation  $z$  in the sequential case. This method is employed to obtain analytically approximation of the model involving fractional derivatives. The study explores into how substrate concentration is affected by various parameter values, including fractional orders. Specifically, it examines how variations in saturation and diffusion parameters affect the normalized current. The study further emphasizes that, as a specific case, the HPM solutions for the reaction/diffusion equation with fractional-order tend to solution for the integer-order model.

## Nomenclature

$\mathbb{C}$	Catalyst.
$S$	Substrate.
$P$	Product.
$\mathbb{C}'$	An immobilized catalyst in its catalytically active state $\mathbb{C}$ .
$K$	Partition coefficient
$K_M$	Michaelis-Menten Constant.
$k_c$	Catalytic constant.
$[SC]$	Substrate-Enzyme complex.
$[PC]$	Product-Enzyme complex.
$D_s$	Substrate's diffusion coefficient.
$D'_s$	The Nernst diffusion layer.
$L$	Polymer layer of thickness.
$s^\infty$	Bulk concentration of substrate.
$\phi$	Thiele modulus.
$\alpha$	Saturation parameter.

## The mathematical formulation of the problem

Consider a thin, uniformly thick layer of electro catalytically active polymer film applied to a conductive  $z$  support surface to form a chemically  $z$  modified electrode. It is assumed that the catalytically active sites within the polymer film are uniformly distributed, thus ensuring a homogeneous reaction environment. It is further presumed that the layer maintains electrical conductivity and that the rate remains in affected by charge percolation through the film. The substrate is regarded as forming the immobilized catalyst with MM kinetics under the following two-step reaction



$$z\mathbb{C}' \xrightleftharpoons{k'_E} \mathbb{C} \quad (2)$$

Where  $\mathbb{C}$  and  $\mathbb{C}'$  stand for the immobilized catalyst's catalytically active state.  $K_M$  is denoted by MM constant. The non-dimensional parameters are used to express the reaction/diffusion equation as follows [4].

$$\frac{d^2w}{d\chi^2} + \frac{n}{\chi} \frac{dw}{d\chi} - \frac{\gamma w(\chi)}{1 + \alpha w(\chi)} = 0 \quad (3)$$

Where,

$$w = \frac{S}{kS^\infty}; \chi = \frac{x}{L}; \alpha = \frac{kS^\infty}{K_M}; \gamma = \phi^2 = \frac{k'L^2}{D_s}$$

With the boundary conditions  $z$

$$k\chi = 0, \quad \frac{dw}{d\chi} = 0 \quad (4)$$

$$k\chi = 1, \quad w(\chi) = 1 \quad (5)$$

Where  $w$  indicates dimensionless concentration substrate, and  $\chi = \frac{x}{L}$  species the distance parameter. The third term is non-linear concentration, often known as Michaelis-Menten kinetics, while the first two terms indicate substrate diffusion inside the polymer matrix.

The constant, which in the cases of planar, cylindrical, and spherical geometry are  $n = 0, n = 1$ , and  $n = 2$ . Now that the normalized current can be written as follows:

$$y = \alpha \left( \frac{dw}{d\chi} \right)_{\chi=1} \quad (6)$$

## A fractional approach.

In terms of the new generalized Caputo-sequential type non-integer derivative sense, the previous model (3) – (6) is reformulated as follows:

$${}^{CS}_0 D_\chi^{2\mu} w(\chi) + \frac{n}{\chi} {}^{CS}_0 D_\chi^\mu w(\chi) - \frac{\gamma w(\chi)}{1 + \alpha w(\chi)} = 0 \quad (7)$$

With the boundary conditions

$$\chi = 0, \quad \frac{dw}{d\chi} = 0 \quad (8)$$

$$\chi = 1, \quad w = 1 \quad (9)$$

Where  ${}^{CS}_0 D_\chi^{2\mu}$  represents Caputo-Sequential derivative with fractional order  $2\mu$ .

## Equilibrium and Stability Analysis

The term "steady-state" in electro active polymer films denotes a state wherein the polymer film exhibits a stable and uniform electrochemical response. During this phase, processes like oxidation or reduction reactions within the polymer film reach equilibrium, leading to consistent values of normalized current, diffusion, or saturation parameters that persist over time.

### The equilibrium point of our model is

$$E^0 = (w^0, Y) = \left( -\frac{1}{(\alpha + \gamma)}, 0 \right)$$

**Theorem 1:**  $z$  The equilibrium of the model (7) is locally asymptotically stable if  $\alpha, \gamma > 0$ . Otherwise unstable.

**Proof.** Consider the Jacobian matrix  $J(E^0)$  given by:

$$J(E^0) = \begin{pmatrix} 0 & 1 \\ -\frac{(\alpha + \gamma)^2}{\gamma} & -\frac{n}{x} \end{pmatrix}$$

To determine its eigenvalues, solve the characteristic equation  $|J(E^0) - \lambda I| = 0$ .

$$\lambda^2 + \frac{n}{x}\lambda + \frac{(\alpha + \gamma)^2}{\gamma} = 0$$

Thus,

$$\lambda = -\frac{n}{2x} \pm \frac{\sqrt{\frac{n^2}{x^2} - 4\frac{(\alpha + \gamma)^2}{\gamma}}}{2}$$

This shows that for  $\alpha, \gamma > 0$ . Therefore, the Eigen values are negative real parts, indicating locally asymptotically stable.

### Model solution by using FHPM [27]

#### Construct the homotopy

$$(1 - p) \left( {}^C_0 D_x^{2\mu} w(\chi) \right) + p \left( {}^C_0 D_x^{2\mu} w(\chi) + \frac{n}{x} {}^C_0 D_x^\mu w(\chi) - \frac{\gamma w(\chi)}{1 + \alpha w(\chi)} \right) = 0$$

$${}^C_0 D_x^{2\mu} w(\chi) = p \left( \frac{\gamma w(\chi)}{1 + \alpha w(\chi)} - \frac{n}{x} {}^C_0 D_x^\mu w(\chi) \right) \quad (15)$$

Using the perturbation technique,  $w$  can be expressed as the series in  $p$  that follows:

$$w(\chi) = w_0(\chi) + p w_1(\chi) + p^2 w_2(\chi) + \quad (16)$$

Substituting (16) into (15) and Equating powers of  $p$ .

$$p^0 : {}^C_0 D_x^{2\mu} w_0(\chi) = 0$$

$$p^1 : {}^C_0 D_x^{2\mu} w_1(\chi) = \frac{\gamma w_0(\chi)}{1 + \alpha w_0(\chi)} - \frac{n}{x} {}^C_0 D_x^\mu w_0(\chi)$$

$$p^2 : {}^C_0 D_x^{2\mu} w_2(\chi) = \frac{\gamma w_1(\chi)}{1 + \alpha w_1(\chi)} - \frac{n}{x} {}^C_0 D_x^\mu w_1(\chi)$$

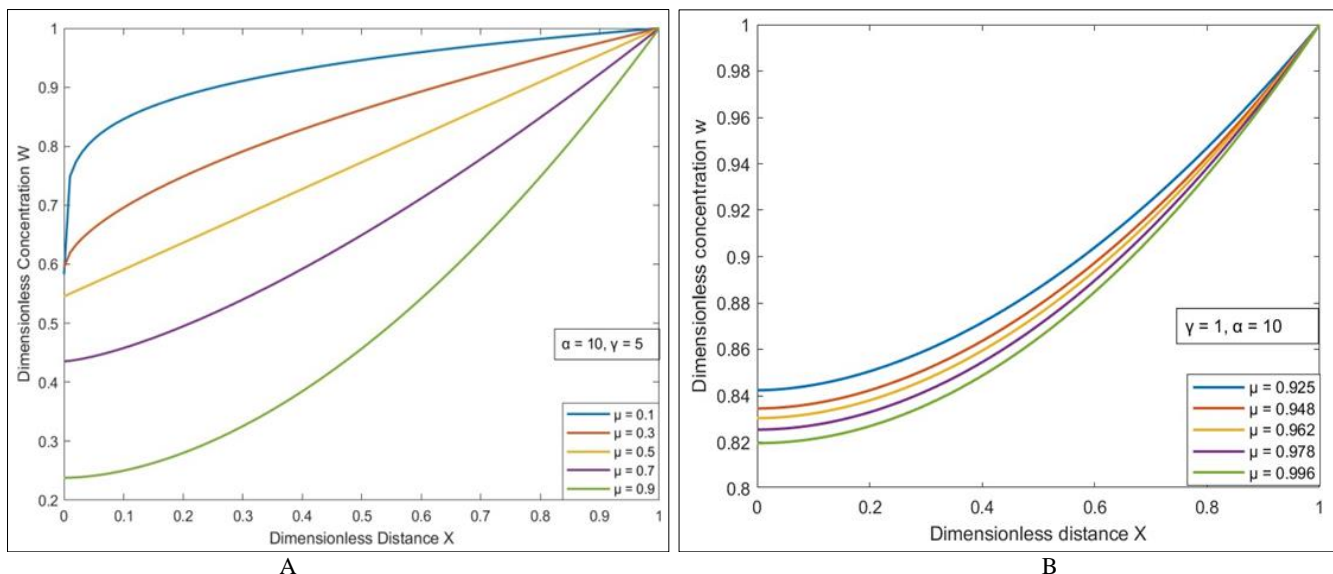
Applying  $J^\mu$  which is inverse of  $D^\mu$  into find  $w_0(\chi), w_1(\chi), \dots$   
 $w_0(\chi) = 1$

$$w_1(\chi) = \frac{\gamma}{(1 + \alpha)\Gamma(2\mu + 1)} \chi^{2\mu} - \frac{\gamma}{(1 + \alpha)\Gamma(2\mu + 1)}$$

Letting  $p \rightarrow 1$  gives therefore,

$$w(\chi) = 1 - \frac{\gamma}{(1 + \alpha)\Gamma(2\mu + 1)} + \frac{\gamma}{(1 + \alpha)\Gamma(2\mu + 1)} \chi^{2\mu} - \quad (17)$$

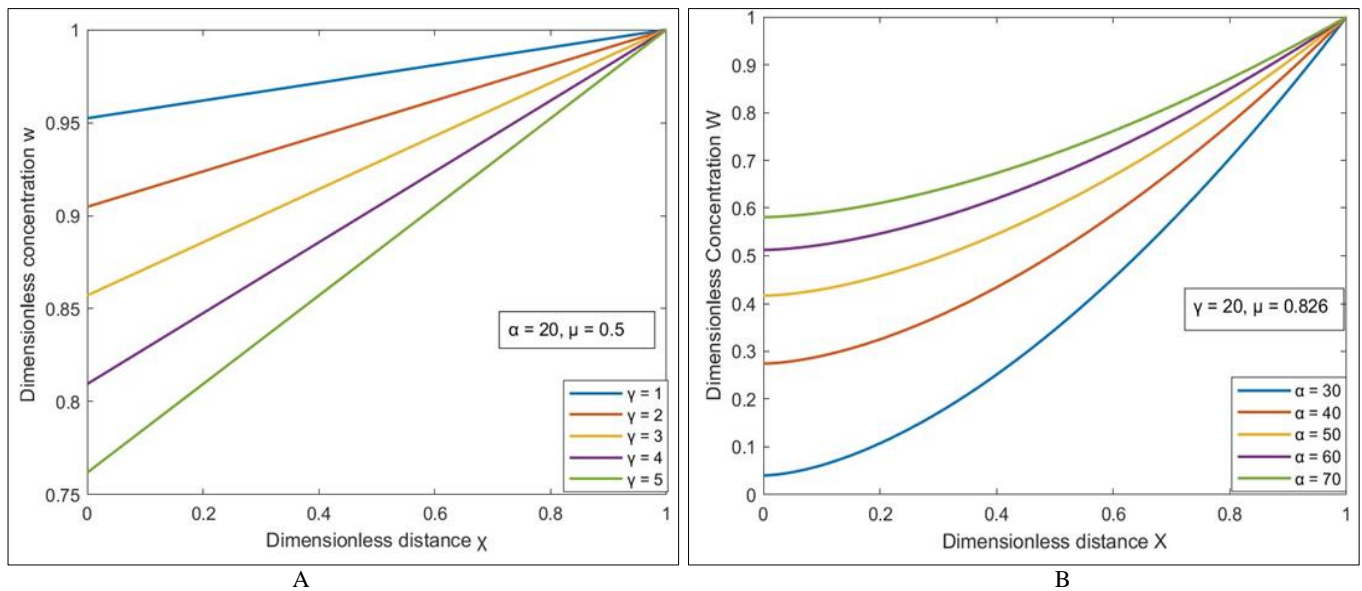
### Graphical analysis



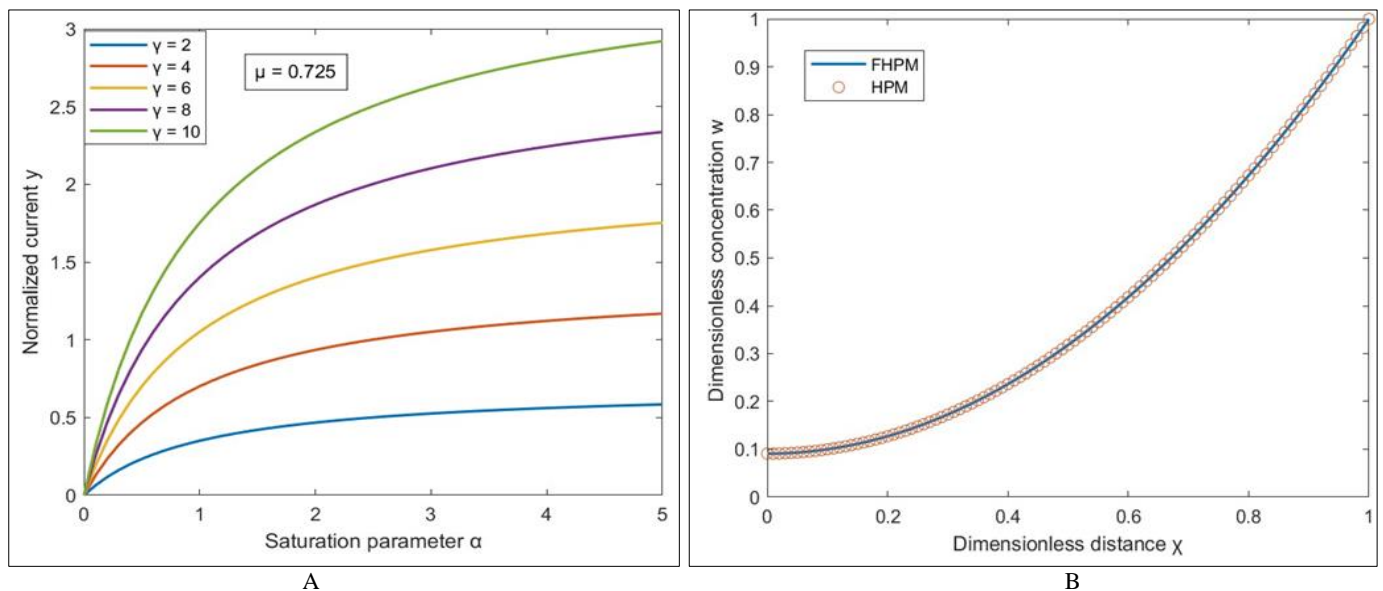
**Fig 1:** Dimensionless distance  $\chi$  versus Dimensionless concentration of substrate  $w(\chi)$  computed using (17), for various order  $\mu$ , and for some fixed values.

In Figures.1 demonstrate the Dimensionless concentration of substrate  $w(\chi)$  for certain values of parameter  $(\alpha, \gamma)$  with different fractional order  $\mu$ . In Figures.2 leads to that as it (a)  $\gamma$  increases the concentration of substrate  $w(\chi)$  on the electrode surface decrease, (b)  $\alpha$  increases the concentration of substrate  $w(\chi)$  on the electrode surface increase. Due to a thin layer, the reaction kinetics accelerate more quickly than the substrate's diffusional transport. Consequently, the reaction is governed by diffusion, resulting in significant

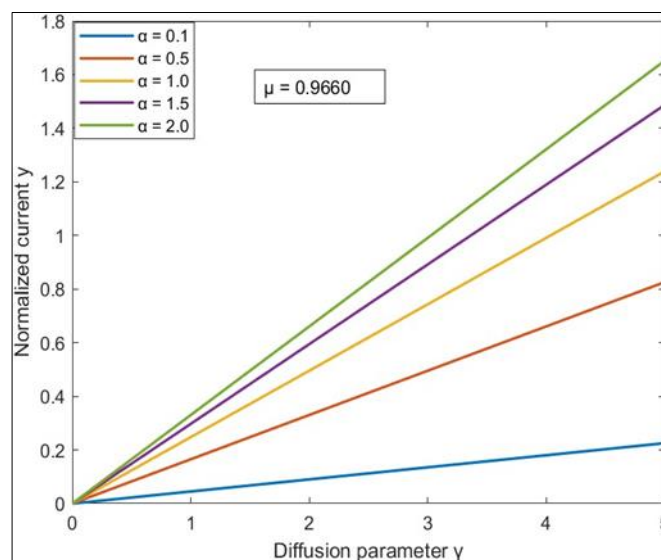
concentration polarization in the film. In Figures. 3 (a) and (b), the plots of dimensionless normalized current  $y, z$  versus diffusion parameter  $\gamma$  / saturation parameter  $\alpha$  consistently show increasing trends in alignment with each other. In Figures.4 shows that the solution of the Caputo-sequential  $z$  fractional differential equation (17), yields the solution  $z$  of the corresponding integer-order derivative as special case  $\mu \rightarrow 1$ .



**Fig 2:** Dimensionless distance  $\chi$  versus Dimensionless concentration of substrate  $w(\chi)$  computed using (17), (a) for different values of  $\gamma$  and for a specific value of  $\alpha$  with the order  $\mu = 0.5$ . (b) for different values of saturation parameter  $\alpha$  and for a given value of  $\gamma$  with the order  $\mu = 0.826$



**Fig 3:** Dimensionless  $z$  normalized current  $y$  versus dimensionless  $z$  saturation parameter  $\alpha$  and diffusion  $z$  parameter  $\gamma$  for several values of other  $z$  parameter



**Fig 4:** According to the particular case  $\mu \rightarrow 1$ , the HPM solution (17), provides the solution (A3).



This model offers a strong framework for applying the reaction-diffusion mechanism in biofuel cells and bioreactors, and it is especially well-suited for amperometric sensors. The model also makes it easier to understand the MM kinetics of enzymes in electrochemical systems and may be modified to improve the performance and design of biosensors for a range of uses, such as environmental monitoring and renewable energy.

## Conclusion

The theoretical model of the electrode system of the steady-state amperometric sensor, which exhibits Michaelis-Menten kinetics, was developed using a second-order non-linear differential equation and then expanded to the Caputo-Sequential fractional differential equation. The non-linear reaction/diffusion equation investigated with approximative analytical solutions, specifically Homotopy Perturbation method, which is an efficient and effective method that can be utilized for fractional derivatives. The influence of various values of the parameter is discussed. The fractional-order model is more reliable than the that has been previously published integer-order model. In addition, we show that in a specific case, the caputo-sequential fractional equation leads to the solution of integer-order case.

## Conflict of Interest

All authors declare that there are no conflicts of interest in this paper.

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## Appendix A

### The HPM of solving second-order integer equation of reaction/diffusion equation (3)

#### Using Homotopy for the equation (3)

$$(1-p) \left( \frac{d^2 w}{dx^2} \right) + p \left( \frac{d^2 w}{dx^2} + \frac{n}{x} \frac{dw}{dx} - \frac{\gamma w(x)}{1+\alpha w(x)} \right) = 0$$

$$\frac{d^2 w}{dx^2} + p \frac{n}{x} \frac{dw}{dx} - p \frac{\gamma w(x)}{1+\alpha w(x)} = 0 \quad (A1)$$

#### Using the perturbation technique

$$w(x) = w_0(x) + pw_1(x) + p^2 w_2(x) + \quad (A2)$$

**Substituting (A1) into (A2) and equating the powers of  $p$**

$$p^0: \frac{d^2 w_0}{d\chi^2} = 0$$

$$p^1: \frac{d^2 w_1}{d\chi^2} = \frac{\gamma w_0(\chi)}{1 + \alpha w_0(\chi)} - \frac{n}{x} \frac{dw_0}{d\chi}$$

$$p^2: \frac{d^2 w_2}{d\chi^2} = \frac{\gamma w_1(\chi)}{1 + \alpha w_1(\chi)} - \frac{n}{x} \frac{dw_1}{d\chi}$$

$$\vdots$$

**Integration with respect to  $\chi$  with the boundary conditions (4) and (5)**

$$w_0(\chi) = 1$$

$$w_1(\chi) = \frac{\gamma}{2(1+\alpha)} \chi^2 - \frac{\gamma}{2(1+\alpha)}$$

Letting  $p \rightarrow 1$  gives therefore,

$$w(\chi) = 1 - \frac{\gamma}{2(1+\alpha)} + \frac{\gamma}{2(1+\alpha)} \chi^2 - \quad (A3)$$