

# On Irreversible Thermodynamic for a New Collision Frequency Model of Boltzmann Equation for a Gas Mixture Influenced by a Centrifugal Force

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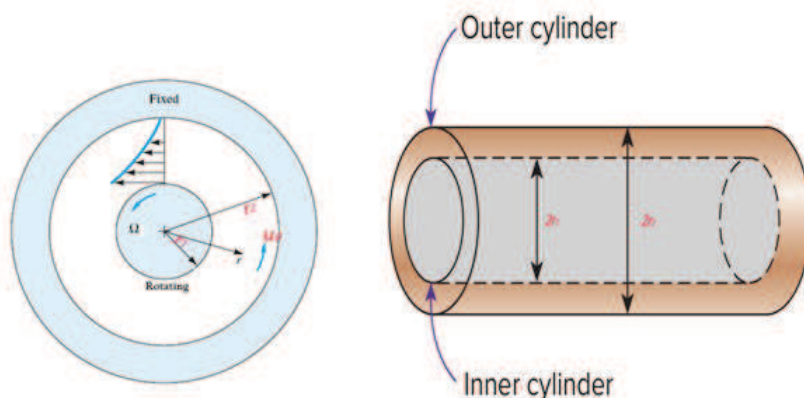
**Abstract:** This paper discussed a new mathematical model of the Boltzmann equation for a gas mixture influenced by a centrifugal force. We do that to study the performance of the particles' non-equilibrium unsteady distribution function of a gas confined between two parallel rigid concentric cylinders. This examination is done in a non-restricted range of Knudsen number and a non-restricted range of a centrifugal Mach number. For this approach, an exact analytical moments equation of the new kinetic mathematical model is presented for two-sided non-equilibrium distribution Maxwellian functions. Our new mathematical model is a significant modification and a considerable development of the BGK (Bhatnagar-Gross-Krook) model of the Boltzmann equation to be appropriate for investigating the effect of the centrifugal force on a neutral gas mixture. The new mathematical model's scientific achievement is that it represents an uncomplicated mathematical model that has no mathematical complication. On the other hand, the mathematical model does not lose any of its generality. The mathematical model formula is citable for any coordinate system. Nevertheless, we will focus here on the mathematical model related to the cylinder coordinate. We shed light upon the new mathematical model satisfaction of the conservation laws of energy, mass, and momentum, thermodynamics second law, and Boltzmann H-theorem. The new mathematical model for a centrifugal force, utilized in the Uranium enrichment process and affecting on the neutral gas mixture between two concentric circular rigid cylinders, is discussed as a significant application for the new mathematical model. We also introduced the irreversible non-equilibrium thermodynamics mathematical formulas of the system related to the new mathematical model for the first time at all. The ratios between the various participations of the internal energy modifications are calculated. The flow of a neutral binary gas mixture of ( $UF_6$  and  $N_2$ ) between rotating cylinders is the first suggested problem enforcement of the new mathematical model.

**Keywords:** Statistical mechanics theorems, Irreversible thermodynamics, Statistical thermodynamics, Nuclear energy generation, Centrifugal force, Unsteady BGK new mathematical model, Uranium enrichment

## 1 Introduction

Uranium enrichment improves the proportion of the fissile isotope U-235 about five- or six-fold from the 0.7% of U-235 obtained in natural. Uranium enrichment is a physical process, often relying on the mass difference between the atoms of the uranium isotopes U-238 and U-235. Currently uranium enrichment processes need uranium to be in a neutral gaseous state, so the compound uranium hexafluoride ( $UF_6$ ) [1]. The neutral gas centrifuge device for separating the isotopes is also called the ultracentrifuge due to the very high speeds involved. Developments of the centrifugation process had made centrifuges practical and economical. The centrifuge consists of a cylindrical chamber (the rotor) turning at a very high speed in a vacuum. Neutral gas is supplied, and the centrifugal force tends to compress it near the outer cylinder. However, the thermal motivation force tends to redistribute the neutral gas molecules throughout the entire volume. Small mass molecules are selected in this effect, and their concentration is higher beside the center axis.

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**Fig. 1:** Two parallel horizontal rigid concentric cylinders. The outer is fixed but the inner one is rotating.

By several means, countercurrent flow of  $UF_6$  neutral gas is decided that tends to carry the heavy and light isotopes to opposite directions of the rotor [2]. The American physicist Jesse Wakefield Beams and his colleagues are the chiefs who demonstrated the centrifugal process of neutral gas isotope separation [3]. Currently centrifuges are routinely utilized in a variety of disciplines such as the pharmaceutical, medical, chemical, mineral, dairy, agricultural, and food industries. Available centrifuge models and configurations seem almost as massive as their applications [4].

In the investigation of the neutral gas centrifuge, it is necessary to calculate the collision frequency of the neutral gas particles as a function of position within the device. That is due to the centrifugal force, which is distributed gas particles' in a very non-consistent performance between the upper cylinder and the lower one. Indeed, examination indicates that while the high-density region near the upper cylinder can be treated as a continuum regime, the region near the lower behaves like a rarefied gas regime. Similarly, this attitude calls for special techniques based upon a Boltzmann kinetic theory description of the gas particles' attitude [5–10]. Pomraning [6] has proposed a useful mathematical model dealing with the centrifugal force that acts on gas in the plane geometry. He used a demonstrate force term in the Boltzmann kinetic equation to simulate the centrifugal effect. L. M. De Socio et al. [7] showed that the comparisons display that the agreement between the simulations and the experiments is excellent in the continuum regime. At the same time, it gives a very good one in the transitional regime. A full review of previous works in the applications of the kinetic theory to the centrifugation process problems can also be found in E.A. Johnson and L. M. De Socio's papers [7–9].

The large magnitude of the Knudsen numbers that happen in rarified gas dynamics is related to the high magnitude of the mean free path or of characterized length minimal value. That is happening in the micro-electro-mechanical systems (MEMS) or Nano-electro-mechanical systems (NEMS) devices. That property gives the Boltzmann kinetic equation an excellent advantage and several modern applications rather than the Navier-Stokes equations [11, 12]. Many papers addressed Boltzmann equation and its applications in many important physical situations such as thermal force and micro gas sensor [13, 14], irreversible thermodynamics and plasma [15–17], sound propagation in rarefied gases [18], oscillatory flow [19, 20], thermal radiation [21, 22], plasma [23], Brownian particles [24], ultra-relativistic heavy-ion collisions [25], photon gas [26], granular fluids [27], electron energy distribution function [28] and other several interested applications [29–32].

This paper investigates the new collision frequency mathematical model of the Boltzmann kinetic equation for a neutral gas mixture influenced by a centrifugal force for studying the performance of the particles' non-equilibrium unsteady distribution function of a gas confined between two parallel horizontal rigid coaxial cylinders. This examination is done in a non-restricted range of Knudsen number and a non-restricted range of a centrifugal Mach number. For this approach, an exact analytical moments equation of the new kinetic mathematical model is presented for two-sided non-equilibrium distribution Maxwellian functions. The moment method [33] with a suitable boundary and initial conditions is employed. The macroscopic characteristics of the neutral gas mixture are examined. The calculation of non-equilibrium distribution function helps discuss the non-equilibrium thermodynamic characteristics of the entire system (the neutral gas mixture particles + the two cylinders). The system's internal energy change is presented.

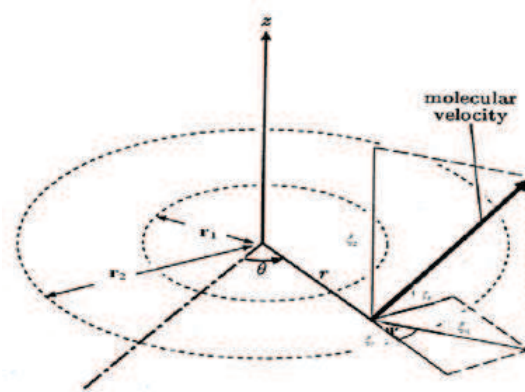


Fig. 2: Cylindrical coordinate systems for concentric cylinders.

## 2 Mathematical and physical problem

We present an unsteady flow of a neutral gas mixture between two illimitable concentric circular cylinders with two radii  $r = r_1$  and  $r_2$  where ( $r_1 < r_2$ ). While the rotate cylinder is the inner one, rotates with an angular velocity  $\omega$ , the fixed cylinder is the outer one. The rotate cylinder generates a centrifugal force ( $m\omega^2r$ ) where  $m$  is the neutral gas atom mass. An analogous constant temperature  $T_S$  is preserved at the surfaces of the cylinders. The cylinders have total momentum, energy accommodation, and diffuse reflection of the incident neutral gas molecules. That occurs with an equilibrium distribution functions  $\varphi_1$  and  $\varphi_2$  at the same temperature  $T_S$ . We focus on a cylindrical coordinate system  $(r, \theta, z)$ , where the  $Oz$  axis coincides with the axis of the cylinders,  $r$  is the distance from this axis, and  $\theta$  is an azimuthally coordinate. The molecular-velocity distribution function  $\varphi(r, \xi_r, \xi_\theta, \xi_z, t)$  obtains the axis-symmetric  $z$ -independent state of a rarefied neutral gas mixture. Here  $\xi_r, \xi_\theta$  and  $\xi_z$  are the orthogonal components of the molecular velocity in the radial, azimuthal, and axial directions, respectively. In the velocity space, we also present a cylindrical coordinate system with an axis parallel to the  $Oz$  axis. Let  $\xi_n$  denote the velocity component that is lying in a plane normal to the cylinders' axis and  $\psi$  be the angle between this component and the radial direction from the axis of symmetry. The formulas relate to the orthogonal velocity components  $\xi_r, \xi_\theta$ , and the polar coordinates of the velocity are:  $\xi_r = \xi_n \sin \psi, \xi_\theta = \xi_n \cos \psi$ . The neutral gas moves along the azimuthal direction, while its radial velocity is zero [10]. The distribution functions fulfilled the kinetic equation with the new modified BGK collision term. The kinetic equation for both neutral gases had the formula [20, 21, 31–35]:

$$\frac{\partial \varphi_A}{\partial t} + \xi \cdot \frac{\partial \varphi_A}{\partial \mathbf{r}} + \frac{\mathbf{F}_A}{m_A} \cdot \frac{\partial \varphi_A}{\partial \xi} = v_{AA} (\varphi_{A0} - \varphi_A) + v_{AB} (\varphi_{B0} - \varphi_A) \tag{1}$$

$$\frac{\partial \varphi_B}{\partial t} + \xi \cdot \frac{\partial \varphi_B}{\partial \mathbf{r}} + \frac{\mathbf{F}_B}{m_B} \cdot \frac{\partial \varphi_B}{\partial \xi} = v_{BB} (\varphi_{B0} - \varphi_B) + v_{BA} (\varphi_{A0} - \varphi_B) \tag{2}$$

where  $v_{AA}, v_{AB}, v_{BB}$ , and  $v_{BA}$  are (gas A- gas A, gas A - gas B, gas B- gas B and gas B- gas A) new modified collision frequencies respectively. We give the new mathematical model formula in the guide of the references [6, 34–38]:

$$\begin{cases} v_{AA} = \frac{n_0}{2} \sqrt{\frac{8KT_S}{\pi m_A}} (\pi d_A^2) e^{-m_w A M_C^2 (1-r^2)}, v_{AB} = \frac{n_0 \mu_{AB}}{m_B} \sqrt{\frac{8KT_S}{\pi m_A}} (\pi d_{AB}^2) e^{-m_w A M_C^2 (1-r^2)} \\ v_{BB} = \frac{n_0}{2} \sqrt{\frac{8KT_S}{\pi m_B}} (\pi d_B^2) e^{-m_w B M_C^2 (1-r^2)}, v_{BA} = \frac{n_0 \mu_{AB}}{m_A} \sqrt{\frac{8KT_S}{\pi m_B}} (\pi d_{BA}^2) e^{-m_w B M_C^2 (1-r^2)} \end{cases} \tag{3}$$

Here  $d_{AB} = \frac{d_A + d_B}{2}$ ,  $\mu_{AB} = \frac{m_A m_B}{m_A + m_B}$ ,  $M_C = \frac{\omega H}{\sqrt{2KT_S}}$ , where  $M_C$  is the centrifugal Mach.  $m_w$  is the molecular weight of the neutral gas atom.  $d_A$ , and  $d_B$  are the molecular diameters of A, and B gas atoms,  $m_A$ , and  $m_B$  are the two masses. Moreover,  $H$  is a characteristic length of the system,  $n_0$  is the neutral gas concentration at rest, and  $\varphi_{\beta 0}$  are the local Maxwellian distribution function denoted by:

$$\varphi_{\gamma 0} = n_0 (2\pi RT_S)^{-\frac{3}{2}} \left( 1 + \frac{\xi_r u_{r\gamma}}{RT_S} + \frac{\xi_\theta u_{\theta\gamma}}{RT_S} \right) \exp\left(\frac{-\xi^2}{2RT_S}\right), \gamma = A \text{ or } B. \tag{4}$$

The BGK model of the Boltzmann kinetic equation contented the energy conservation law, mass conservation law, momentum conservation law, the second law of non-equilibrium thermodynamic, and the Boltzmann H-theorem. Then

our new mathematical model also contented the conservation of energy, conservation of mass, conservation of momentum laws, the second law of non-equilibrium thermodynamic, and the Boltzmann H-theorem. Thus, our new mathematical model had the same dependent on equilibrium distribution functions and non-equilibrium distribution functions as the BGK model had. Let us write the solution of equations (1) and (2) in the form [34,35]:

$$\varphi_{\gamma}(\vec{r}, \vec{\xi}, t) = \begin{cases} \varphi_{1\gamma} = \frac{n_0}{(2\pi RT_S)^{\frac{3}{2}}} \left(1 + \frac{\xi_r u_{r1\gamma}}{RT_S} + \frac{\xi_{\theta} u_{\theta 1\gamma}}{RT_S}\right) e^{-\frac{\xi^2}{2RT_S}} : \alpha \leq \psi \leq \pi - \alpha \\ \varphi_{2\gamma} = \frac{n_0}{(2\pi RT_S)^{\frac{3}{2}}} \left(1 + \frac{\xi_r u_{r2\gamma}}{RT_S} + \frac{\xi_{\theta} u_{\theta 2\gamma}}{RT_S}\right) e^{-\frac{\xi^2}{2RT_S}} : \pi - \alpha \leq \psi \leq 2\pi + \alpha \end{cases} \quad (5)$$

where  $u_{r1\gamma}$  and  $u_{\theta 1\gamma}$  are eight unknown functions of time  $t$  and the distance variable  $r$  where  $\gamma = A$  or  $B$  and  $i = 1$  or  $2$ . Using Grad's moment method [39–41], by multiplying equations (1) and (2) by  $M_j(\xi)$  and integrating overall values of  $\xi$ , we acquire the transfer equations for neutral gas A:

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \int M_j(\xi) \varphi_A d\underline{\xi} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \int M_j(\xi) \xi_r \varphi_A d\underline{\xi} \right) - \frac{1}{r} \int \xi_{\theta}^2 \varphi_A \frac{\partial M_j(\xi)}{\partial \xi_r} d\underline{\xi} + \\ & \frac{1}{r} \int \xi_r \xi_{\theta} \varphi_A \frac{\partial M_j(\xi)}{\partial \xi_{\theta}} d\underline{\xi} - \left( \int (\omega r^2) \varphi_A \frac{\partial M_j(\xi)}{\partial \xi_r} d\underline{\xi} \right) = \\ & v_{AA} \int M_j(\xi) (\varphi_{A0} - \varphi_A) d\underline{\xi} + v_{AB} \int M_j(\xi) (\varphi_{B0} - \varphi_A) d\underline{\xi} \end{aligned} \quad (6)$$

and the transfer equations for neutral gas B:

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \int M_j(\xi) \varphi_B d\underline{\xi} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \int M_j(\xi) \xi_r \varphi_B d\underline{\xi} \right) - \frac{1}{r} \int \xi_{\theta}^2 \varphi_B \frac{\partial M_j(\xi)}{\partial \xi_r} d\underline{\xi} + \\ & \frac{1}{r} \int \xi_r \xi_{\theta} \varphi_B \frac{\partial M_j(\xi)}{\partial \xi_{\theta}} d\underline{\xi} - \left( \int (\omega r^2) \varphi_B \frac{\partial M_j(\xi)}{\partial \xi_r} d\underline{\xi} \right) = \\ & v_{BB} \int M_j(\xi) (\varphi_{B0} - \varphi_B) d\underline{\xi} + v_{BA} \int M_j(\xi) (\varphi_{A0} - \varphi_B) d\underline{\xi} \end{aligned} \quad (7)$$

$M_i$  is a function of the velocity. The integrals give the moment  $\overline{M}_i$  of  $M_j(\xi)$  over the velocity distance from the relation [39–41],

$$\overline{M}_i = \int M_i(\xi) \varphi_{\gamma} d\underline{\xi} = \int_{\alpha}^{\pi-\alpha} \int_0^{\infty} \int_{-\infty}^{\infty} M_i \varphi_{1\gamma} \xi_n d\xi_z d\xi_n d\psi + \int_{\pi-\alpha}^{2\pi+\alpha} \int_0^{\infty} \int_{-\infty}^{\infty} M_i \varphi_{2\gamma} \xi_n d\xi_z d\xi_n d\psi \quad (8)$$

$$M_i = M_i(\xi), i = 1, 2 \text{ and } d\underline{\xi} = \xi_n d\xi_z d\xi_n d\psi.$$

### 3 The nonequilibrium thermodynamic characteristic of the system

The issues of irreversible processes persist a great interest [40–44]. It has numerous applications in various branches of science. We should consider that the unsteady state non-equilibrium thermodynamic characteristics of the system are discussed under the effectiveness of a centrifugal force. Entropy per unit mass  $S$  is defined as:

$$S_{\gamma}(r, \theta, t) = - \int \varphi_{\gamma} \ln \varphi_{\gamma} d\underline{\xi} = - \left( \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \varphi_{1\gamma} \ln \varphi_{1\gamma} d\underline{\xi} + \int_{-\infty}^{\infty} \int_0^{\infty} \int_{-\infty}^{\infty} \varphi_{2\gamma} \ln \varphi_{2\gamma} d\underline{\xi} \right), \quad (9)$$

The entropy flux vector

$$\vec{J}_{\gamma}(r, \theta, t) = - \left( \int_{-\infty}^{\infty} \int_0^{\infty} \int_{-\infty}^{\infty} \vec{\xi} \varphi_{1\gamma} \ln \varphi_{1\gamma} d\underline{\xi} + \int_{-\infty}^{\infty} \int_0^{\infty} \int_{-\infty}^{\infty} \vec{\xi} \varphi_{2\gamma} \ln \varphi_{2\gamma} d\underline{\xi} \right), \quad (10)$$

Accordingly, the entropy production has the form [44–50]:

$$\sigma_{\gamma}(r, \theta, z, t) = \frac{dS_{\gamma}(r, \theta, z, t)}{dt} = \frac{\partial S_{\gamma}(r, \theta, z, t)}{\partial t} + \vec{\nabla} \cdot \vec{J}_{\gamma}(r, \theta, z, t) \geq 0 \quad (11)$$

The non-equilibrium thermodynamic forces are [21–23, 38]:

$$X_{1\gamma} = \frac{\Delta r}{n_{\gamma}} \nabla_r n_{\gamma}, \quad X_{2\gamma} = \frac{\Delta r}{u_{r\gamma}} \nabla_r u_{r\gamma}, \quad X_{3\gamma} = \frac{\Delta r}{u_{\theta\gamma}} \nabla_r u_{\theta\gamma}, \quad X_{4\gamma} = F_{C\gamma} = -M_c^2 m_{\gamma} r, \quad (12)$$

here  $M_c = \frac{\omega r_1}{\sqrt{2RT_S}}$  is the centrifugal Mach number,  $m_\gamma$  is the gas atom mass, and  $\Delta r$  is the thickness of the layer adjacent to the inner cylinder in units of the mean free path, the distance between two collisions of the neutral gas particles, in dimensionless form.

calculating the non-equilibrium thermodynamic forces and the entropy production for each gas component, we can acquire the kinetic coefficients  $L_{ij\gamma}$ . We can do that from the relationship between the entropy production and the non-equilibrium thermodynamic forces, via the form [42, 44]:

$$\sigma_\gamma(r, \theta, z, t) = \sum_i \sum_j L_{ij\gamma} X_{i\gamma} X_{j\gamma} = (X_{1\gamma} X_{2\gamma} X_{3\gamma} X_{4\gamma}) \begin{pmatrix} L_{11\gamma} & L_{12\gamma} & L_{13\gamma} & L_{14\gamma} \\ L_{14\gamma} & L_{22\gamma} & L_{23\gamma} & L_{24\gamma} \\ L_{31\gamma} & L_{32\gamma} & L_{33\gamma} & L_{34\gamma} \\ L_{41\gamma} & L_{42\gamma} & L_{43\gamma} & L_{44\gamma} \end{pmatrix} \begin{pmatrix} X_{1\gamma} \\ X_{2\gamma} \\ X_{3\gamma} \\ X_{4\gamma} \end{pmatrix} \geq 0 \quad (13)$$

These formulas arise due to the thermodynamics second law itself [41, 44–50]. The necessary and sufficient conditions for  $\sigma_\gamma(r, \theta, z, t) \geq 0$  are fulfilled by the determinant  $|L_{ij\gamma} + L_{ji\gamma}| \geq 0$ , and all its principal minors are non-negative too. Another restriction on  $L_{ij\gamma}$  was established on (1931) by Onsager. He was able to demonstrate the symmetry property denoted by  $L_{ij\gamma} = L_{ji\gamma}$ , which is called the Onsager-Casimir reciprocal relations.

The Gibbs’s formula for the internal energy modifications applied to the system  $dU_\gamma$  is as follows:

$$dU_\gamma(r, \theta, z, t) = dU_{S\gamma} + dU_{V\gamma} + dU_{F\gamma}. \quad (14)$$

The internal energy modifications due to the change of the extensive variables, such as entropy  $dU_{S\gamma}$ , volume  $dU_{V\gamma}$ , centrifugal force  $dU_{F\gamma}$  [38, 44], as follows:

$dU_{S\gamma} = T_S dS_\gamma$  and  $dU_{V\gamma} = P_S dV_\gamma, dU_{F\gamma} = -M_c^2 m_\gamma r dr$ . Here  $dV_\gamma = \frac{-dn_\gamma}{n_\gamma^2}$ ,  $P_S = n_S T_S$ ,  $dS_\gamma = \frac{\partial S_\gamma}{\partial r} \delta r + \frac{\partial S_\gamma}{\partial \theta} \delta \theta + \frac{\partial S_\gamma}{\partial z} \delta z + \frac{\partial S_\gamma}{\partial t} \delta t, dn_\gamma = \frac{\partial n_\gamma}{\partial r} \delta r$ . Thus, we had finished the wholly presented of the new mathematical model and its non-equilibrium thermodynamics mathematical formulas as well as its related equations.

## 4 Conclusion

We had introduced a new mathematical model formula of the Boltzmann kinetic equation collision frequency, which is suitable for a neutral binary gas mixture when it is influenced by a centrifugal force. That new mathematical model can be applied in the centrifugation processes. It is also suitable for many various industrial applications. Also, new irreversible thermodynamic mathematical formulas are presented according to our new model. We investigated the new mathematical model that is satisfied with the conservation laws of energy, mass, momentum, thermodynamics second law, and Boltzmann H-theorem. The new mathematical models for a centrifugal force utilized in the Uranium enrichment process and affecting on a neutral gas mixture between two concentric circular rigid cylinders, are discussed as a significant important application for the new mathematical model and its related new mathematical equations.

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## Conflict of Interest

The authors declare that they have no conflict of interest.

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