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Oscillatory Flow As A Means Of Enhanced Species Separation: A Three Dimensional Time-accurate Cfd Analysis

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OSCILLATORY FLOW AS A MEANS OF ENHANCED SPECIES SEPARATION: A THREE DIMENSIONAL TIME-ACCURATE CFD ANALYSIS

by

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B.S. Metropolitan University, 1999

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in the Department of Mechanical, Materials and Aerospace Engineering in the College of Engineering and Computer Science at the University of Central Florida Orlando, Florida

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ABSTRACT

A fluid that contains species in the presence of a concentration gradient generates unusual phenomena when it is forced into pulsatile motion. For example, each species in the fluid has an enhanced mass transport due to pure molecular diffusion. This enhancement takes place even if there is no net total flow over a cycle of the pulsatile motion. When more than one species in dilute amounts is present in an otherwise pure fluid, called a carrier, each species is transported at a different rate thereby causing a partial separation of the species. This idea traces back to hyperventilation studies done over 40 years ago and to the implementation of the technology in hospital environments to provide life-support for patients under anesthesia. However, it is only in recent years that the underlying physics of oscillatory flow as applied to mass transfer have been understood and this may lead to promising application of the technique to novel means of enhancing separation in life support applications and for detection purposes.

In this thesis, results from three-dimensional time accurate studies carried out using the commercial computational fluid dynamics code FLUENT are presented. These results simulate the separation of CO\textsubscript{2} from H\textsubscript{2} in an N\textsubscript{2} environment (carrier). The model consists of two reservoirs/mixing chambers, an oscillating piston wall, and a connecting tube. Several cases are carried out reporting on separation enhancement as a function of the Womersley number and the ratio of tidal displacement to connecting tube diameter. Unlike previous studies which were undertaken using asymptotic analysis, the present models and results incorporate full entrance effects and 3D interactions. Results of this
study will be useful as a guide for the design and miniaturization of an oscillating device for species separation in further research projects at the University of Central Florida.

Observations showed that a molar fraction increase occurs during the species transport in the presence of a thermal boundary layer. This was accompanied by an imposed external forced temperature condition on the surface of the cylinder to create thermal diffusion, also known as the Soret or thermal diffusion effect, which refers to the separation of mixtures in a temperature gradient as means of change on the concentration gradient of the species ratio.

Calculations were performed to analyze the effect of the heat transfer on the molar fraction of the species at a specific region of the model, called the measurement point. Various mathematical models and correlations were incorporated into a MATLAB computer code that predicted the concentration of the species in an entire cycle after steady state is reached and data can be exported from FLUENT.
Dedicated to my Husband, Dad, Mom, Karen, Oscar and Fernando,

Dr. Alain Kassab and Dr. Eduardo Divo
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LIST OF ABBREVIATIONS

$c_j$: Mass concentration

$C_j$: Axial ass concentration of a component $j$

$c_p$: Specific heat at constant pressure, $J/kg \, K$

$d$: Diameter of the cylinder, device, $m$

$D_T$: Thermal diffusion coefficient, $m^2/s$

$D_j$: Mass diffusion coefficient for component $j$ of a multi-component mixture, $m^2/s$

$D_h$: Hydraulic diameter, $m$

$Ec$: Eckert Number, $V^2 / c_p \cdot \Delta T$

$G$: Mass flux, or mass velocity, $\rho \cdot V$

$h$: Heat Transfer coefficient, or convection conductance, $W/m^2.k$

$J_j$: Diffusion flux vector, $\rho_j (u_j - V), kg/m^2.s$

$K_T$: Thermal diffusion ratio, $D_T/D_j$

$L$: Length of the cylinder, $m$

$m_j$: Mass fraction of component $j$, $kg/kg$ of mixture, $\rho_j / \rho$

$M_j$: Molar weight, $kg/mol$

$Nu$: Nusselt number, $h \cdot d / k$

$Pr$: Prandlt Number, $v / \alpha$

$q"$: Heat flux, heat – transfer rate at surface per unit area, $W/m^2$

$Q$: Mass transfer rate, $kg/s$

$r$: Radius of the cylinder, also found as $a$ in 1-D equations, $m$
Re: Reynolds Number, \( \rho V d / \mu \)

\( R_i \): Net rate of production of species \( i \) by chemical reactions

\( Sc \): Modified Schmidt number, \( v_{mix}/D_j \)

\( S_i \): Rate of creation of species \( i \) by addition from the dispersed phase plus any user-defined sources

\( S_t \): Stanton number, \( h / Gc \)

\( T_s \): Fluid temperature at the surface, \( K \)

\( T_m \): Mixed mean temperature at the surface, \( K \)

\( u_m \): Mean velocity of species \( j \), equivalently a mass-weighted velocity, \( m/s \)

\( u_c \): Assigned velocity at any desired point, \( m/s \)

\( V \): Axial velocity vector, \( \vec{V} \), \( m/s \)

\( V \): Velocity magnitude, \( m/s \)

\( \dot{w}_j \): Mass of each component \( j \), per unit volume and time product of species reactions

\( Wr \): Womersley number, \( r(\omega/\nu)^{1/2} \)

\( X_j \): Molar fraction of component \( j \)

\( Y_j \): Mass fraction of component \( j \)

\( \alpha \): Thermal diffusivity, \( k / \rho \cdot c_p \cdot m^2/s \)

\( \rho \): Fluid density, \( kg/m^3 \)

\( \rho_j \): Partial density of species \( j \), \( kg/m^3 \)

\( \eta \): Similarity parameter; independent variable in Blasius and other similarity solution equations
\( \zeta \): Dependent variable in Blasius equation, \( u / u_\infty = \zeta ' (\eta) \)

\( \Gamma \): Ratio of effective mass fluxes, \( (G_{\text{effect}})_{\text{lightest}} / (G_{\text{effect}})_{\text{heavier}} \)

\( \mu \): Dynamic viscosity, \( N \) s / \( m^2 \)

\( \nu \): Kinematic viscosity, \( \mu / \rho \), \( m^2 / s \)
A fluid that contains species in the presence of a concentration gradient generates unusual phenomena when it is forced into pulsatile motion. For example, each species in the fluid has an enhanced mass transport due to pure molecular diffusion. This enhancement takes place even if there is no net total flow over a cycle of the pulsatile motion. When more than one species in dilute amounts is present in an otherwise pure fluid, called a carrier, each species is transported at a different rate thereby causing a partial separation of the species\textsuperscript{1-5}. This idea traces back to hyperventilation studies done over 40 years ago and to the implementation of the technology in hospital environments to provide life-support for patients under anesthesia. However, it is only in recent years that the underlying physics of oscillatory flow as applied to mass transfer have been understood and this may lead to promising application of the technique to novel means of enhancing separation in life support applications and for detection purposes.

The purpose of this thesis is to create a three-dimensional computational fluid dynamics, CFD, analysis, which simulates an oscillatory separator of non-reacting chemical species driven by piston motion. This model simulates a physical device located at the Chemical Engineering Department at the University of Florida that consists of two reservoirs connected by an oscillatory cylinder that imparts the pulsatile motion. The separation in the experiment is thus driven by cylinder motion at certain amplitudes and frequencies, and an analytical solution can be obtained\textsuperscript{3-5} to produce curves for the ratio of the species molar flow at the tube centerline as a function of frequency of oscillation assuming an incompressible flow in an infinitely long cylinder, neglecting entrance and
end effects. On the other hand, the time accurate CFD simulation reported in this thesis incorporates entrance and exit effects as well as three dimensionality of the problem using a hexahedral grid replicating most of the structure of the original device, while the pulsatile motion is imparted by a sinusoidal moving wall in one of the reservoirs.

The moving wall is initialized and the time-accurate CFD model is ran through the transient regime. After a periodic sustained regime is reached, the ratios of the radial concentrations are analyzed. The fundamental purpose of the CFD simulation approach is to compare the molar fraction of species obtained after the steady state regime is reached when pure diffusion and when the oscillatory flow driven by the motion of the piston respectively drove the behavior of the species transport accounting for 3-D effect at the entrance and exit regions of the tube as well as developing boundary layers and the improvement of the molar fraction when the Soret effect is imposed as a temperature boundary condition along the cylinder. The corresponding temperature is written either as a constant or as a position function.

Comparisons are made for several ratios of tidal displacements of the tube lengths as a function of Womersley number to provide a guide for design and implementation of physical separation devices. The commercial solver FLUENT was used for all CFD modeling. The 3-D time-accurate CFD study reveals improvement in the separation of the species under oscillatory motion, confirming theoretically predicted tuning frequencies. However, the level of improvement is found to be less than theoretically predicted due to 3-D entrance effects.
CHAPTER TWO: LITERATURE REVIEW AND BACKGROUND

Many different studies have been carried out on the species transport either for liquids or gases. Increases in mass transfer rates can be achieved by the correlations between the velocity and concentration fields over those due to molecular diffusion alone; this makes the pulsating motion attractive in diverse separation applications. The phenomenon of transport enhancement of species was initially investigated by Taylor\(^7\) and Aris\(^8\) in studies of axial dispersion in steady flows. Results in steady laminar flows indicated that an increase in the axial species dispersion occurs. Other effects were found in oscillating flows by Bowden\(^9\). Harris and Goren\(^1\) studied the mass transfer between two containers by orders of magnitude. Kurzweg and Jaeger\(^3\) first showed the existence of a “tuning” characteristic of mass diffusion by oscillating flows and suggested its use for gas separation. Recent studies by Wilhelm, Rice and Bendelius\(^10\) also carried out variations in the concentrations by using pulsating flow coupled with a temperature gradient in a bed packed with absorbent particles. Many types of separation processes have been utilized for the purification of gases, in particular air. Investigators have employed a variety of separation technologies whose designs are customized to mission duration and integration with on-board systems. Most methods require the use of chemical reagents, absorbent materials, or some version of membrane technology. The embodiment of the new technology proposed in this study capitalizes on the ability of properly tuned oscillating flows to achieve efficient and effective separation of chemical species. The proposed technology is relatively complex, and it requires none of the above-mentioned separation technologies that require continuous regeneration or
refreshing; computational time use will be the major issue instead. However, it could also be applied to separation of other organic contaminants from air; oscillating flows can be used as a purely mechanical way to assist in the air revitalization process by removing both fine submicron particles and unwanted organics that may be present in the air. This will help sustain a habitable environment needed for advanced life support. Because oscillating flows are a mechanical means of separation, re-supply of filters, membranes, or other physical-chemical materials are not needed. Although this process may not fully replace standard separations methods for removal of fine particles and organics, oscillating flows hold great promise as a precursor to other separation techniques. This will help reduce the load and increase the longevity for processes that require re-supply of materials.

In addition, this can be applied to the separation of particles, the separation of electrolytes in solutions, the separation of isotopes, the maintenance of inert blanket gasses in hermetically preserved compartments, and to enhance heat transfer.

The applications of the oscillation motion of species are the motivation of this study and can be summarized as:

- Separation of gaseous species is technologically important, for instance separation of CO₂ or other species from air is important to the space program.
- Periodic flow uses purely mechanical (non-chemical) means to assist in separation: enhanced diffusion.
- Potential applications to separation of aerosols in air for a pre-concentrator to assist in detection of chemical/biological aerosols.
- Potential application to separate particles such as flake obscurant materials from aerosols.
2.1 Mechanism of the Separator of the Species

Species separation was originally envisioned in space missions as a means of air revitalization. This study is immediately applicable to separation of carbon dioxide from helium in space environments. The physics of the problem involves multiple length pipes and time scales. To understand the physics consider first the transport of a dilute species in a carrier gas in a long cylindrical pipe between two large reservoirs as it is shown in figure 1.

![Figure 1: Separation of Species Model](image)
Pure diffusion occurs due to an axial concentration gradient: species migrate to carrier side or right reservoir. The transport of species is characterized by its molecular diffusion coefficient, $D_j$, through Ficks’ Law.

If a time periodic pressure gradient, such as an external force, is imposed to the gases, an oscillatory flow will be established. Periodic flow uses purely mechanical (non-chemical) means to assist in separation giving as a result the enhancement of the diffusion and separation of species\textsuperscript{45}. The original device shown in figure 2 is located in the facilities of the Chemical Engineering Department at the University of Florida. Components of this mechanism are described in detail in figure 3.

Figure 2: Overall View of the Existing Oscillating Flow Apparatus (University of Florida, Gainesville)
Figure 3: Description of the model (University of Florida, Gainesville)

This mechanism has been used to create curves to calculate the ratio of the species concentration at diverse tidal displacements and frequencies. The description of the functionality of this oscillatory device is explained based on the convective flow motion for two species: carbon dioxide and helium in figures 4 and 5.

\[ \text{CO}_2 \quad \text{He} \]

Figure 4: First half of the cycle

In the first half of the oscillation cycle, figure 4, a hydrodynamic boundary layer forms and causes radial concentration gradients generating a movement of the species contained in the mixture from core to wall. The lighter species, in this case the He, will tend to move faster than the CO\(_2\) and larger amounts of He will be displaced farther from the centerline where the maximum velocity is attained.
In the second half of the oscillation cycle, figure 5, the hydrodynamic boundary layer forms in reverse and causes again radial concentration gradients forcing the diffused species to migrate from the wall to the core.

At the start of the first half of the next oscillation cycle, figure 6, the species in the fast moving core of the tube (larger amounts of CO$_2$) is convected down the tube core and again diffuses towards the wall due to high concentration gradients.

Figure 7 represents the axial oscillation of the fluid in motion while figure 8 is the net enhanced axial mass transfer of the carrier. The enhanced effective diffusion occurs when the motion of the cylinder or moving wall is:
1. In forward motion of the hydrodynamic boundary layer and diffusion from high concentration core to low concentration at the wall.

2. In reverse motion of the hydrodynamic boundary layer and diffusion back from wall to core.

![Figure 8: One cycle for species (dilute in carrier and non-interacting)](image)

The axial convective motion and the radial diffusion are the outcome of the oscillating motion, which is precisely the point of interest in this study: to know how this coupling phenomenon can make any difference when more than one species with different molar weights are incorporated in the model, and how the tidal ratio of species concentration improves as a result of it.

### 2.2 Mass Transfer by Convection and Mass Transfer by Diffusion

Formulation of diffusion and thermal conduction is similar. The similarity arises because the thermal conduction involves the diffusion of heat down temperature gradient and the mass transport involves the diffusion of mass down concentration gradients. Given the total mass flux vector \( \mathbf{G} \, (\text{kg} / \text{m}^2.s) \), and the total velocity vector \( \mathbf{V} \, (\text{m/s}) \) related as:

\[
\mathbf{V} = \mathbf{G} / \rho
\]
For multi-component concentration gradients, the convected mass flux of component \( j \), defined as the flux of \( j \), attributed to bulk fluid motion is: \( G_{\text{conv},j} = m_j \), and the diffusion mass flux of component \( j \), \( m_j = \rho_j / \rho \), is therefore:

\[
G_{\text{diff},j} = G_{\text{tot},j} + G_{\text{conv},j}
\]

\[
\sum m_j = 1 \quad \text{and} \quad \sum G_{\text{tot},j} = \sum G_{\text{conv},j} = G \sum m_j = 1
\]

Then:

\[
\sum G_{\text{diff},j} = 0
\]

This means that, even if there is no bulk motion of the fluid, it is still possible to have diffusion, but the summation of various components will be zero.

As a result, the rate of diffusion of a single component of a mixture \( G_{\text{diff}} \), is a function of the concentration gradient of that component and other potential gradients acting on the system, such as temperature, concentration or pressure gradients of the other components. Then, Ficks’ law is defined for a mixture as:

\[
\sum G_{\text{diff},j} = -\rho D_j \nabla m_j
\]

For a gas, the diffusion of component \( j \), in the mixture under the influence of both concentration and temperature gradients corresponds to the follow relation:

\[
\sum G_{\text{diff},j} = -\rho D_j (\nabla m_j + \frac{M_1 M_2}{M^2} K_T \nabla \ln T)
\]

The second term on the right-hand side of the equation 5 is derived to express the thermal diffusion. The thermal diffusion ratio \( K_T \), is derived from kinetic theory of
gases\textsuperscript{11}. In some applications, this value is a constant if a mean temperature is considered\textsuperscript{12} as $K_T = D_T/D$. The ratio of thermal diffusion is also called the Soret coefficient where it is partially inserted to ensure good thermalization and avoid boundary convection. Typical values of $K_T$ range between 0.001 to 0.01 for gases or simple electrolytes\textsuperscript{13}, but calculation to establish the importance of this effect in typical boundary layer flow has been studied.

Furthermore, the form of the thermal diffusion ratio is also found as polynomial functions, user-defined functions, or empirically based composition dependent expressions as:

$$D_{T,j} = -2.59 \times 10^{-07} T^{0.659} \left( \sum_{j=1}^{N} M_{j,d}^{0.511} X_i - Y_i \right) \left( \sum_{j=1}^{N} M_{j,d}^{0.511} X_i \right)$$

Where $X_i$ is the mole fraction and $Y_i$ is the mass fraction of any component $i$. This formulation is directly extracted from FLUENT\textsuperscript{14}. In time accurate solutions, this coefficient is calculated during the iteration process for every component $i$, by equation 6, until steady state regime solution is reached in the CFD simulation.

### 2.3 Binary Boundary Layers

The mass concentration of any component $j$, is:

$$c_j = \frac{\rho_j}{\rho}, \quad \rho_j = \lim_{(\Delta V \rightarrow 0)} \frac{\Delta m_j}{\Delta V}$$

With $\sum_j c_j = 1$, and $\rho_j$ is the partial density.
At any point, the velocity of a component can be different from the others. Simplification reduces to the calculation of a mean value in order to characterize the flow. The mean velocity concept is introduced as:

\[ \bar{u}_m = \sum_j c_j \bar{V}_j \]  

Where the mean velocity vector \( \bar{u}_m \), is equivalently a mass-weighted velocity. This velocity is also found in the momentum and thermal energy equations. 

Furthermore, the mass conservation equation for component \( j \), is read as:

\[ \text{div}(\rho_j \bar{u}_j) = \dot{w}_j \]  

In the case of chemical reaction, the mass of each component \( j \), per unit volume and time product of species reactions is \( \dot{w}_j \) [20].

The conservation of mass for the summation of all components is given by:

\[ \text{div}(\rho \bar{V}) = 0 \]  

If there is any difference in the concentration of the mixture as expected, relative velocities of each component or species \( j \), associated with the mass-weighted velocity, are present in the equations. Hence the mass flows with the coordinate system related with the mass-weighted velocity, then, the diffusion flux vector \( J_j \), is obtained as:

\[ J_j = \rho_j (\bar{u}_j - \bar{V}) \]  

For instance, the concentration of species 1 is governed by the continuity equation as:

\[ \rho \frac{\partial c_1}{\partial t} + \rho \left( \bar{V}_j \frac{\partial c_1}{\partial x_j} \right) = -\frac{\partial J_{1j}}{\partial x_j} + \dot{w}_i \]
In the case of carbon dioxide and helium no chemical reactions \( \dot{w}_j \), are taken into consideration in this study.

The diffusion law delivers the relation between the diffusion flux vector \( J_j \), and the concentration and temperature fields\(^{16}\). For two-component mixtures:

\[
J_j = -\rho D_{12} [\nabla c_1 + K_T c_1 (1 - c_1) \nabla \ln T]
\]

In this equation, the diffusion effects due to pressure and the diffusion due to volume forces by gravitational fields are also neglected.

The diffusion law defines a coupling effect between heat conduction and mass transfer. It describes the effects of the concentration gradients and the temperature gradients over mass transfer. The concentration gradient corresponds to the Ficks’ diffusion law which is associated with the Fourier law of heat conduction.

The second term, thermal diffusion, gives rise to an additional mass transfer due to temperature gradients, which changes the mass transfer of each component. The diffusion coefficient \( D_j \), is independent of the concentration and it is considered constant for each of the species.

Assuming mixture of ideal gases, the enthalpy of the mixture is: \( i = \Sigma c_j i_j \). Enthalpies, \( i_1 \) and \( i_2 \), are absolute values. In a binary mixture, physical properties depend on the temperature, the pressure, and the concentration. The dependence can be exceptionally small, especially in asymptotic methods. The effects of diffusion on heat conduction are usually neglected in some applications\(^{17}\).

Then the governing equations for a system are written as:
Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho V_j) = 0$$  \hspace{1cm} (13)

Conservation of linear momentum equation:

$$\frac{\partial}{\partial t} (\rho V_i) + \frac{\partial}{\partial x_j} (\rho V_j V_i) = \rho f_i - \frac{\partial \rho}{\partial x_i} + \frac{\partial \tau_{ji}}{\partial x_j}$$  \hspace{1cm} (14)

Conservation of energy equation, one component $j=1$:

$$\frac{\partial}{\partial t} (\rho c_p T) + \frac{\partial}{\partial x_j} (\rho c_p V_j T) = \beta T \left[ \frac{\partial p}{\partial t} + V_j \frac{\partial p}{\partial x_j} \right] + \tau_{ji} \frac{\partial V_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( k \frac{\partial T}{\partial x_j} \right)$$

$$+ \frac{\partial}{\partial x_i} \left\{ \rho D_{12} (i_1 - i_2) \left[ \frac{\partial c_1}{\partial x_i} + K_i c_1 (1 - c_i) \frac{\partial \ln T}{\partial x_i} \right] \right\}$$  \hspace{1cm} (15)

Through an iteration process, each of the equations are solved until sustained solution is reached meaning that values of density $\rho$, concentration $c$, and mass transfer $Q$, can be calculated as mean values.\textsuperscript{19} As it is expected, changes on the diffusivity are found either to increase or to decrease. Changes also depend on the species properties, and their molar weight.

In addition, changes in temperature are evaluated as well. The purpose is to observe how variations in the species concentrations due to thermal gradients correspond to any improvement on the tidal concentration ratio of the species. The analysis of the merged moving thermal boundary layer combined with axial concentration gradients and the radial diffusion due to convective flow is the focus of this study. Next section explores the notion behind the temperature changes and how it could affect the species transport.
2.4 Thermal Diffusion - Ludwig-Soret effect

If an external force acts on the system through any boundary conditions, such as temperature, pressure, or concentration and mass heat flux\textsuperscript{21} occurs as consequence. This phenomenon is also known as the Ludwig-Soret effect that refers to the separation of mixtures in the presence of temperature gradients. Since its discovery by Ludwig (1856) and the first investigations in liquid mixtures by Soret (1879), the effect has been subject to study. Relevant applications are effectively implemented on polymer and petrol reservoir characterization and accumulation of uranium\textsuperscript{21-24}.

When thermal diffusion is allowed, rearrangement of the system occurs as it is shown in figure 9. Even though the effect has not been much studied, it has emerged due to a physical reason: the system organizes itself in such a way that heat is transported most effectively with minimum entropy production\textsuperscript{24-27}.

![Figure 9: Illustration of the Soret effect](image)

As a result, the heavier or more strongly interacting species achieves increasing velocity, decreasing diffusivity and rearranging in cold regions of the system\textsuperscript{23}.

For a binary mixture, in time-dependent solutions, the variation of the concentrations for species $j$, in space and time, is governed by the changes on the thermal
field by an increase or decrease of the diffusivity and velocity of their molecules at different amplitudes and frequencies. The improvement on concentration profiles are found by numerical integration in an entire cycle after steady state regime is reached in the solution.
CHAPTER THREE: RESEARCH METHODS

The following sections describe the elaborated design that permits assessing the validation of the Computational Fluid Dynamics solution, CFD, with the corresponding results from the 1-D Asymptotic Analytical approach\textsuperscript{4-5}. The maximum separation of the species due to different effects is, in the end, the main goal of the study.

In conjunction with the design of the prototypes, parameters and correlations are carefully calculated and standardized in order to properly compare between results. To evaluate and analyze them, the variables are chosen to be dimensionless for further research purposes. Formulations, procedure, and coding are explained for the asymptotic solution while the modeling and simulation from the computational analysis are described step by step to ensure the approximation to the overall existing apparatus\textsuperscript{1-5}. Furthermore, the effects of the change in temperature at the boundaries are taken under consideration as a way to search for improvement on the tidal concentration ratio and its optimal points.

3.1 Numerical Models and Correlations for Asymptotic Analytical Solution

The analytical results are based on solutions reported in\textsuperscript{1-5}. The model includes an incompressible flow through a long cylinder oscillating between two infinitely large reservoirs.
The motion is driven by a position function, then, the volumetric flow rate in a cross-section is written as:

\[ q = \frac{1}{2} A_o \omega \pi a^2 \cos(\omega t) = \frac{1}{4} A_o \omega \pi a^2 (e^{i\omega t} + e^{-i\omega t}) \]  

Where \( A_o \) is the amplitude, \( \omega \) is the frequency, and \( a \) is the radius of the cylinder. The axial velocity vector \( V \) is governed by:

\[ \frac{\partial V}{\partial t} = \nu \left( \frac{\partial^2 V}{\partial r^2} + \frac{1}{r} \frac{\partial V}{\partial r} \right) - \frac{q}{2} \]

The tidal displacement or amplitude \( A_o \), needs to be sufficiently small, so that the condition of zero net convection between the cylinder ends is maintained. This way, an infinite cylinder model neglects end effects, developing flow, and concentration boundary layers in the entrance region, and imposes a mean linear axial concentration gradient:

\[ (C_2 - C_1)/L \]

where \( L \) is the distance separating the two tanks and the \( C_1 \) and \( C_2 \) are the concentrations of the any component at positions 1 and 2. A periodic sustained velocity field is assumed such that:

\[ V = \hat{V} e^{i\omega t} + \tilde{V} e^{-i\omega t} \]

Then:

\[ V = w A_o \left\{ \begin{array}{l} 1 - J_o \left( \frac{\alpha r}{a} \right) \\ J_o(\alpha) \end{array} \right\} e^{i\omega t} + \left\{ \begin{array}{l} 1 - J_o \left( \frac{\alpha' r}{a} \right) \\ J_o(\alpha') \end{array} \right\} e^{-i\omega t} \]
Where:

\[
\alpha = \left( \frac{-iwa^2}{\nu} \right)^{\frac{1}{2}} \quad \text{and} \quad \alpha' = \left( \frac{iwa^2}{\nu} \right)^{\frac{1}{2}}
\]

It is necessary to recall that the 1-D asymptotic solution is referenced as boundary driven (as opposed to pressure driven derived by Kurzweg\(^3\), existing mechanism and the developed model for the Computational Fluid Dynamics, CFD, presented in this study).

Assuming no-slip boundary condition and finite velocity at \(a = 0\), the separation of the species will occur whenever the ratio, \(\Gamma\), between the effective mass fluxes of the lightest species over the other one is equal to 1. For instance, helium and carbon dioxide correspond to the formulation: \(\Gamma = (G_{\text{effe}})^{\text{He}} / (G_{\text{effe}})^{\text{CO}_2}\). Otherwise, separation is not possible. On the other hand, the rate of separation depends on the values of the axial concentration, \(C_i\), the ratio, \(\Gamma\), and the modified Schmidt number, \(S_c\). The rate, at which separation of the species occurs, for the case when molecular weights of the components are comparable to each other, is approximated by the following correlations\(^3\) in figure 10,

\[
S_c = \frac{\nu_{\text{mix}}}{D_j}
\]

![Figure 10: Schematic Analysis for Increments in the Species Diffusivity into carrier, N2](image)

- \(S_c = 0.1\) \quad \text{The lightest species, He}
- \(S_c = 10\) \quad \text{The heaviest species, CO}_2

A MATLAB code was implemented to compute results from the analytical solution obtained through asymptotic expansions of Bessel functions defining the axial
velocity. The concentration for each species $j$, far from the end is governed by the unsteady diffusion-advection equation as:

$$\frac{\partial c}{\partial t} + V \frac{\partial c}{\partial x} = D \left( \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial x^2} \right)$$

Finally, the increase of the rate of mass transfer is found to be proportional to the oscillatory Reynolds number, $Re = \omega a^2 / v$, and the Schmidt number, $Sc$, which means that at any Reynolds number, the increment on the mass transfer rate changes as the square of the pulse amplitude given by the following relation 4-5:

$$\frac{Q - Q_{diff}}{Q_{diff}} = \sqrt{2} \frac{Sc}{(Sc^2 - 1)} \left( \frac{\omega a^2}{v} \right)$$

In addition, a correspondence between piston driven and boundary driven flow is established to compare CFD results to those provided by equation 21.

A measurement point for this approximation is located at the center of the cylinder where end effects can be neglected 4-5. Figure 11 shows the boundary driven flow as it is taken for coding.
Several experiments have been performed with the mechanism located in the facilities of the University of Florida and from the output of the MATLAB code which contains the formulation described above in order to determine each species effective concentration. Tidal ratio of mass transfer is found providing those results are the comparison point between the One Dimensional Asymptotic Analytical solution and the Computational Fluid Dynamics simulation outcome.

3.2 Description of the CFD Model

The device consists of two reservoirs connected by a cylinder. Each reservoir is a rectangular box with an inlet and outlet. The pulsating effect is generated at the wall of the left-hand reservoir, and it is modeled by a sinusoidal motion of the piston wall. Dimensions and some properties are provided in figure 12.
To accomplish separation of species, the moving cylinder is substituted by a moving wall in one of the extremes as it is shown in figure 12. The model requires creating the volume that simulates as much as possible the original device, which is one of the biggest challenges of this study.

3.2.1 CFD Grid Generation

The model volume was meshed in a multi-block structured hexahedral grid with a number of 281,880 cells, 864,080 faces, and 300,690 nodes. The mesh was clustered near the sidewalls to accommodate the accurate modeling of the boundary layers, see figures 13 to 15.
Figure 13: 3D section of the device used in the CFD Simulation

Figure 14: Sketch of a 2D section of the device used in the CFD Simulation

Figure 15: Sketch of a 3D section of the device used in the CFD Simulation
3.3 Initial Solution without the Oscillatory Wall

The starting point was to obtain the solution from FLUENT for the species without using the moving wall; this was motivated by the fact that the experimental apparatus is initialized with certain pre mixture. The apparatus contains a fan in each reservoir that kept the mixture homogeneous. After steady state is reached due to pure diffusion of the species, the device is ready to begin receiving the effect of oscillating motion.

In the CFD, the equations are solved for $N - 1$ species, where $N$ is the total number of fluid phases of the chemical species present in the system. Since the mass fraction of the species must sum to unity, the $N^{th}$ mass fraction is determined as one minus the sum of the $N - 1$ solved mass fractions. To minimize numerical error, FLUENT requires the species to be organized in descending order of mass fractions; the last species to report in the list has to be the carrier. Then, the $N^{th}$ species should be selected as that species with the overall largest mass fraction. The continuity equation for each species $i$, is recast in the following form:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \bar{V} Y_i) = -\nabla \cdot \bar{J}_i + R_i + S_i$$  \hspace{1cm} (22)$$

Here, $R_i$ is the net rate of production of species $i$ by chemical reactions and $S_i$ is the rate of creation by addition from the dispersed phase plus any user-defined sources.

In this case, only the diffusion of He and CO$_2$ in N$_2$ (carrier) was taken into account in the problem, without neglecting any chemical reactions or user-defined sources.
The diffusion of CO$_2$ is less than that of H$_e$. This was expected because of the difference between the diffusion coefficients of the two species. See figures 16 and 17. In the analysis, the center of the cylinder was a measurement point of the concentrations. For this case the ratio of concentration between the CO$_2$ and H$_e$ was 0.189435; while none of the species had reached the outlet, pressure-outlet, at the right reservoir. This was
calculated by taking the mass-weighted average ratio of concentration of CO$_2$ with respect to H$_2$ at the center of the cylinder. This result is then divided by the molecular weight ratio of 11.

This is the configuration that the oscillating motion will be applied to. The values provided above are taken as the initial values of tidal concentration ratio of the species in further graphs for a frequency value of 0.00 Hz.

### 3.4 Oscillatory Piston Model for CFD Formulation

In order to incorporate the motion on the CFD model, two different approaches in FLUENT were considered to set the motion of the wall in terms of a sinusoidal position.

#### 3.4.1 First Approach: Moving Wall

The first attempt to solve this problem proved to be unsuccessful. The moving wall option of FLUENT was used by defining a user-defined function (UDF). The macro DEFINE_PROFILE was used in the code of the UDF to define the equation of motion at the left-hand wall. After the UDF was written, the boundary conditions at the left-hand wall were set. This proved to be unsuccessful because the moving wall did not function as expected in FLUENT. The results showed the species within the reservoirs moving constantly to the right. The fluid did not behave the way expected and the method proved to be inaccurate. The motion of the fluid should have been oscillatory to reflect the system behavior. In addition, the grid needed to deform with the fluid to obtain an oscillatory motion of both the fluid and grid. In order to obtain the desired motion of the model, a different approach was required. In short, moving wall cannot be used where the
wall has a motion normal to itself; FLUENT will neglect any normal component of wall motion that it is specified. Then, the dynamic mesh option is the only possible option that generates the accurate motion of the boundary on the existing system, and in the end, the separation of species.

3.4.2 Second Approach: Dynamic Mesh

The dynamic mesh model in FLUENT can be used to model flows where the shape of the domain is changing with time due to motion on the domain boundaries. The motion can be prescribed or unprescribed and the subsequent positions are determined based on the solution at the current time. The updated volume mesh is handled automatically by FLUENT at each time step based on the new positions of the boundaries. To use the dynamic mesh model, a starting volume mesh and the description of the motion of any moving zones in the model must be provided. Remeshing is not allowed for hexahedral cells; instead, a layering option is used. FLUENT allows describing the motion using either boundary profiles or user-defined functions. A UDF incorporates C programming language with FLUENT’s macros to assign specific equations of motion corresponding to the problem.

The description of the motion must be specified on face or cell zones. If the model contains moving and non-moving regions, these regions should be identified by grouping them into their respective face or cell zones in the starting volume mesh that is generated. Furthermore, regions that deform due to motion on their adjacent regions must also be grouped into separate zones in the starting volume mesh. For this problem, both the oscillating wall and fluid need to be declared as deforming in a specific zone. While the
oscillating wall is a rigid body zone, the fluid is a deformed one. In the zones, the UDF is attached to the moving face.

### 3.4.3 User-Defined-Function: Dynamic Mesh Code

The UDF created for the problem involves a CG_MOTION routine. This macro in FLUENT allows the oscillatory grid movement of a face. In addition, different commands to send and receive information from the host to nodes\(^{19}\) are required for computational parallelization. The user-defined function written to model the oscillatory motion of the left-hand wall is:

```c
#include "udf.h"
DEFINE_CG_MOTION(piston, dt, vel, omega, time, dtime)
{
    Thread t; /*is the pointer to the structure that stores*/
    real A= ; /* Assign amplitude*/
    real H= ; /* Assign frequency*/
    real \(\omega = 2. \pi \times H\); /*Calculate the omega*/
    real v = A*\(\omega \times \sin(\omega \times \text{time})\); /*Calculate velocity*/

    /* reset velocities . The linear and angular velocities are returned to FLUENT by overwriting the arrays vel and omega, respectively*/
    NV_S (vel, =, 0.0);
    NV_S (omega, =, 0.0);

    /* obtain the thread pointer for which this motion is defines */
    t = DT_THREAD (dt);

    /* compute velocity */
    v = A*\(\omega \times \sin(\omega \times \text{time})\);
    vel[0]= v;
}
```

Then the solution associated with this code will improve in the motion of the wall and the changes of the grid points. For instance, the new configuration in time will be found as shown in the following figures 18 though 20.
An example of the grid motion with $\frac{A_0}{L} = 0.2$ is shown in figures 18 through 20.

A frequency of 0.2 Hz was chosen and the complete cycle of the oscillating wall took 5 seconds to complete.
3.4.4 Define-Profile Function: Temperature Boundary Condition Code

Imposed surface temperature conditions along the length of the cylinder are the factor that generates the Soret effect. This parameter is considered as constant and also as a position function. For the cases where the temperature is considered a constant, the boundary condition can be applied directly as value on the boundary condition panel. However, a define-profile function needs to be created to be able to impose the temperature boundary condition as a position function as a boundary condition as follows:

#include <stdio.h>
#include "udf.h"

DEFINEPROFILE(temperature, thread, position)
{
    face_t f;
    /* f is the pointer to the structure that stores */
    real x = 0.67 + position;   /* Initial position */
    begin_f_loop(f, thread)    /* Iteration process */
    {
        F_PROFILE(f, thread, position) = 74.626 * x + 350;
        /* Example of derived position function */
    } end_f_loop(f, thread)
}

Figure 21 shows the imposed temperature boundary condition along the length of the cylinder.

![Temperature Distribution - Define-Profile Code at the Cylinder](image_url)

Figure 21: Temperature Distribution - Define-Profile Code at the Cylinder
3.5 Boundary Conditions

The boundary conditions defined in this section are the reference values, referred to as standardized values in previous sections.

- The pulsating motion is governed by the following function:

  \[ X(t) = -A_o \cos(\omega t) \]

- Therefore, the corresponding derivative in time yields the speed as:

  \[ V(t) = A_o \omega \sin(\omega t) \]

- Constant Properties:
  - Specific Heat: \( c_p = 1006 \text{ (J/kg K)} \)
  - Thermal conductivity, \( k = 0.0454 \text{ (W/mK)} \)
  - Dynamic viscosity, \( \mu = 1.7200\text{e-05 (kg/m s)} \)

- Diffusion Coefficients:
  - He in \( \text{N}_2 \) = 0.000710 \( \text{(m}^2/\text{s)} \)
  - \( \text{CO}_2 \) in \( \text{N}_2 \) = 0.000165 \( \text{(m}^2/\text{s)} \)

- Range of frequencies: \( f = 0.2 \text{ to } 1.6 \text{ Hz} \)

- Range of amplitudes, \( A_o = 5\%, 7\% \text{ and } 10\% \) of the length of the cylinder, which has a constant value of 1.34 m.

It is important to mention that previous research on this topic is guides to narrow the range of the frequencies and amplitudes to be considered\textsuperscript{1-5}. Calculations of the amplitudes vary according to cross-section area of the oscillating surface. Recall, in the case of the 1-D asymptotic solution, the cylinder is the moving boundary while the left-
hand wall of the device is the moving surface in the Computational Fluids Dynamic, CFD model.

3.6 Test Matrix

Since the beginning of the research, a total of 72 cases with different amplitudes and frequencies were tested using the dynamic mesh model. Also, six amplitudes were chosen and varied in comparison to the total length of the cylinder. At the beginning of the research, amplitudes were chosen to be enormous, so observations of the effective movement of the model and the transport phenomenon were not possible to assess. Nevertheless, the amplitudes of 5%, 7%, 10% of the length of the cylinder were chosen to ensure the validation of this model either for the analytical or the experimental data. In order to guarantee consistency with the analytical model which involves cylinder motion rather than piston motion, a relation is derived to convert those percentages in terms of the oscillatory wall, see figure 22.

Figure 22: 2-D Sketch – Piston Wall - Amplitude Calculation
\[ A_1 \Delta x_1 = A_2 \Delta x_2 \]

For instance, if the displacement is 10% of the cylinder length, \( \Delta x_2 = 0.1L \), and the reservoir to piston area ratio \( A_1/A_2 = 50 \), then \( \Delta x_1 = 0.002L \) and \( A_o = 0.001L \).

An average of six different frequencies is tested for each of the selected amplitudes. The frequencies vary from 0.2 Hz to 1.6 Hz depending on the amplitude to be assigned. The tidal ratio of the species concentration is plotted versus the non-dimensional parameter Womersley Number, \( Wr \):

\[ Wr = \frac{d}{2} \sqrt{\frac{\omega}{\nu}} \]

At the end, calculations from both, One Dimensional Asymptotic solution and CFD solutions for the tidal ratio of the species concentration is expected to approach the curve shown in figure 23.

![Figure 23: Ratio of the Total Mass Transfers for CO2-He System](image)

Figure 23: Ratio of the Total Mass Transfers for CO2-He System
The point at which the tidal ratio reaches the highest value in the Y-axis is called the optimal point, see figure 23. This corresponds to the value of frequency and amplitude at which the maximum separation occurs.

The validation of results will be achieved when

- Total mass transfer increases for both species with increasing $\omega$.
- There are crossover points where mass transfer of one species overtakes the other, see figure 24.
- Existence of optimal frequency.

![Figure 24: Mass Transfer vs. Frequency for a He-CO2 Binary System with N2 carrier](image)

Figure 24: Mass Transfer vs. Frequency for a He-CO2 Binary System with N2 carrier

The reason for using this no dimensional parameter instead of frequency, $\omega$ (rad/sec), is that the model is also under consideration for high dimension reduction. The idea of miniaturization of this device is part of the motivation for further research in this project. Then, tidal ratio and Womersley number are the fundamental parameters in the analysis.

The reference measurement point was located at the outlet, in the right-hand reservoir shown in the figure 12. The mass fraction in one cycle was calculated
numerically using the mid point rule in order to obtain the amount of mass that crossed this section as a function of time; sustained periodic solution is required for all calculations. In addition, two more points of study were located at the center and the outlet of the first reservoir. Monitoring mass conservation during cycles also verified results. Figure 25 shows the cycles graphically. The data extracted from FLUENT was the mass-weighted average for the corresponding species \( H_e \) and \( CO_2 \). The test matrix was composed by the values of frequencies and amplitudes shown in table 1.

![Figure 25: Sinusoidal function - Amplitude calculation by \( X(t) \)](image)

<table>
<thead>
<tr>
<th>( \omega ) (Hz)</th>
<th>( \omega ) (rad/s)</th>
<th>Womersley Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>0.300</td>
<td>1.88497</td>
<td>2.64836</td>
</tr>
<tr>
<td>0.350</td>
<td>2.19913</td>
<td>2.86056</td>
</tr>
<tr>
<td>0.400</td>
<td>2.51329</td>
<td>3.05807</td>
</tr>
<tr>
<td>0.450</td>
<td>2.82745</td>
<td>3.24357</td>
</tr>
<tr>
<td>0.500</td>
<td>3.14161</td>
<td>3.41902</td>
</tr>
<tr>
<td>0.600</td>
<td>3.76993</td>
<td>3.74535</td>
</tr>
<tr>
<td>0.800</td>
<td>5.02658</td>
<td>4.32476</td>
</tr>
<tr>
<td>0.900</td>
<td>5.65490</td>
<td>4.58710</td>
</tr>
<tr>
<td>1.000</td>
<td>6.28322</td>
<td>4.83523</td>
</tr>
<tr>
<td>1.200</td>
<td>7.53987</td>
<td>5.29673</td>
</tr>
<tr>
<td>1.400</td>
<td>8.79651</td>
<td>5.72112</td>
</tr>
<tr>
<td>1.600</td>
<td>10.05316</td>
<td>6.11613</td>
</tr>
</tbody>
</table>
3.6.1 Test Matrix: Thermal Diffusion

The selection of the frequency and amplitudes to provide the validation of the Soret effect were maintained to ensure proper comparisons between results.

The characteristic curve to be found should approximate those in figures 23 and 24. However, the optimal point could result in smaller or larger values of frequencies, as the values of the tidal ratio of concentration are expected to increase or decrease as well. In the end, the purpose of this last approach is to try to improve the separation of the species by achieving to increase the optimal point at any frequency and amplitude. For this task, the variation of the temperature on the surface of the cylinder will be assigned as constant values and position functions.

At first, the cylinder walls are maintained at a constant temperature 100K higher than the inlet temperature of the flow into the reservoir. Also extreme values of changes in temperature, $\Delta T$, were considered in order to verify if the model adjusts to the Soret effect theory in a short simulation process.

The variation on the temperature is considered either increasing or decreasing along the surface of the cylinder. The changes in temperature, $\Delta T$, are maintained to 100K. Therefore, two linear functions are used in the model as Define-Profile functions:

- For increasing temperature:
  \[ T(x) = 74.626x + 350 \]  \(23\)

- For decreasing temperature:
  \[ T(x) = -74.626x + 350 \]  \(24\)
CHAPTER FOUR: RESULTS AND DISCUSSIONS

The initial consideration is that just due to diffusion in the system H\textsubscript{2} is going to diffuse more than the CO\textsubscript{2} in a ratio of almost four. Furthermore, the ratio of the tidal concentration is expected to reach an optimal point and this point is expected to be displaced to higher frequency values as the amplitude gets smaller.

In order to assess the validation of the CFD model, this has to approximately coincide with the asymptotic solution. To compare and analyze results between 3D numerical predictions and 1D asymptotic solution, three different amplitudes were considered: 5%, 7%, and 10% tidal displacement to tube length ratios. The corresponding range of frequencies was set from 0 – 10 rad/s for each amplitude ratio. A plot of the mass flow rates of the two species as a function of Womersley number is shown in figure 26, revealing an increase in mass flow rate (kg/s) with frequency. Notice that the CO\textsubscript{2} mass transfer curves are significantly higher than the H\textsubscript{2} curves due to the molecular weight ratio of 11 between the two species.

![Figure 26: Mass Transfer vs. Womersley number for CO\textsubscript{2} – H\textsubscript{2} system with N\textsubscript{2} carrier](image_url)

Figure 26: Mass Transfer vs. Womersley number for CO\textsubscript{2} – H\textsubscript{2} system with N\textsubscript{2} carrier
Close examination of the corresponding molar flow rates (kmol/s), see Figure 27 to 29, reveals two cross-over points as predicted theoretically, thus confirming a tuning frequency where maximum separation is achieved.

Figure 27: Illustration of crossover with a tidal displacement of 5% of L

Figure 28: Illustration of crossover with a tidal displacement of 7% of L
The molar ratios of the two species at the outlet of the right-hand reservoir are provided in figures 30 to 32 showing an optimal point for all three values of tidal displacement to tube length ratios. The agreement of the 3-D numerical model with 1-D theory is remarkable in that the optimal tuning frequency is computed essentially to be the same. The magnitude of the gain is however predicted to be less in the 3-D model, and this is expected as the 3-D model accounts for entrance effects of the developing hydrodynamic and concentration boundary layers, while the 1-D model assumes fully-developed flow. Moreover, the 3-D model accounts for the effects of the losses due to flow exiting in a sudden expansion and solves for the concentration gradient while the 1-D analytical result assumes a constant axial concentration gradient between two well-mixed tanks. As such, it is indeed expected that the actual enhancement should be less than predicted theoretically.
For this project, a total of three frequencies were taken under consideration to analyze the Soret effect at the curve corresponding to 7% amplitude to tube length ratio.
As it was described before, the changes of the surface temperature were imposed as constant and as position functions. The time required to obtain asymptotic solutions is about 30 minutes.
Furthermore, time accurate results involve highly CPU-intensive computations even through parallelization. As a result, the frequencies to be studied are chosen around the optimal points obtained in the previous analyses. Mass flow rate is also analyzed and will provide important information to explain how the Soret effect generates variations on the ratio of the species molar concentrations. Based on the thermal gradients created due to the imposed temperature changes along the surface of the cylinder, the results shown on figures 33 and 34 display the changes obtained in the concentration of the species.

![Figure 34: Mass Flow of CO₂](image)

### 4.1 Increasing Temperature Function

For the case in which the temperature function has a positive slope, the mass flow rate of the species increase tremendously as the Womersley number increase. However,
the increment of the mass flow rate of the H\textsubscript{2} is larger than the mass flow rate of the CO\textsubscript{2}. In theory, the lighter species is driven under the effect of the high temperatures which means that the H\textsubscript{2} in terms tries to reach the zone of higher temperatures while the heavier species will be under the influence of external sources and convective terms in the energy equation. This effect is coupled with the effect of the thermal boundary layer on the species transport. The changes due to the boundary layer are also shown. However, the concentration ratio of the species decreases. It can be seen from figures 33 and 34 can be seen that the convective effects are very small in contrast with the behavior of the species product of thermal gradient effects, which can be interpreted as a reduction in the concentration of the heavier species. Different results can be obtained if the species is not exposed to thermal diffusion for the steady state regime. As a result, it is obvious that the convective effect is very small with respect to the thermal gradient effect on the ratio of the species concentration. Values of the species concentration do not show any improvement. However, the main purpose of the device is separation of the species as a way to obtain as much CO\textsubscript{2} as possible on the second reservoir. This is a goal that is achieved.

4.2 Decreasing Temperature Function

Differences are found in the case where the temperature decreases as a function of position along the cylinder (from left to right). The difference is that the variation changes from convex to concave on the species mass flow rate. This behavior is very different from the positive slope temperature results, particularly for the H\textsubscript{2}. However, the effect of a negative slope, decreasing temperature on the boundary of the cylinder, has the
opposite effect on the species transport. The lighter species tends to increase its concentration gradient at the beginning of the cylinder. As the temperature decreases, $H_e$ concentration decreases. One more time, the theory is confirmed. The thermal gradient effect on the concentration of the species imposes significant differences on the results. Figures 33 and 34 show how the $CO_2$ mass flow rate decreases. This behavior is expected due to the variation on the thermal boundary layer. The coupling effect of the thermal boundary layer and the oscillating wall does not occur. As a result the species reaches the second reservoir with smaller mass flow rate values even though the frequency increases. Furthermore, diffusivity increases, but the effect is not enough for any improvement on the species concentration at the second reservoir. Results on the mass flow rate can be different if the inlet temperatures are changed, if the starting point is varied with the activation of the thermal diffusion, and possibly, if higher values of the amplitude are taken in consideration.

4.3 Constant Temperature

Finally, the constant temperature case is analyzed. For the purpose of this study, just one frequency is reviewed. The corresponding value is taken where the optimal point is achieved. Validation of the Soret effect can be inferred from figures 33 and 34. Important results are found for a constant temperature on the cylinder $100K$ higher than the flow inlet temperature. An improvement of the tidal ratio of the species is observed. However, it is not as high as the one found without imposing thermal diffusion. The results of constant temperature could be also subject to changes in inlet boundary conditions.
Figure 35: Molar Ratio Comparison of CO$_2$ to He

The molar ratio of the species is shown in figure 35. None of the different forms of the Soret effect improve on the tidal ratio of the species concentration in comparison with the original curve from previous analyses. Recalling that the thermal gradients vary the concentration gradient by the increase or decrease of the diffusion of the species, it is important to bring up the variations on thermal diffusion coefficient with respect to the different temperatures imposed at the boundary. For a constant temperature equal to 200K constant, see figure 36, it was found an increment in the helium and carbon dioxide thermal diffusion coefficients: the helium achieves an increment of 60% of the original value, while the carbon dioxide increases by 33% as it was expected. Even though the helium reaches higher diffusivity values, the concentration ratio of two the species is maintained values above unity, see figure 35.
For higher temperatures (400K), see figure 37, the results are different. As the temperature increases, both species reach higher velocities, which means that the radial diffusion occurs faster and the axial diffusion. This obviously suggests a substantial increment of the concentration of the species due to the moving hydrodynamic boundary layer.
Nevertheless, the thermal diffusion also causes accumulation of the concentration of the heavier species in the coldest sides of the model due to the thermal boundary layer at higher temperatures. Therefore, the heavier species, carbon dioxide, is under two opposite effects. The thermal diffusion coefficient for the carbon dioxide reduces 7% from its original value, while the helium increases by 13%. These results explain the behavior of the tidal ratio observed in figure 35. Further research can be conducted to obtain improvements in the ratio of the species concentration at lower temperature changes.
CHAPTER FIVE: CONCLUSION

A three-dimensional time-accurate CFD model has been developed to simulate a species separation device whose mechanism is based on oscillatory flow. The results compare well with those from a simplified 1-D analysis confirming the validity of the method to enhance species separation by incorporating a time-accurate sustained solution.

![Graph showing molar ratios of CO₂ to He as a function of tidal displacement ratio and Womersley number for 3D CFD model](image)

Figure 38: Composite of molar ratios of CO₂ to He as a function of tidal displacement ratio and Womersley number for 3D CFD model

Figure 38 is a summary of the analytical and CFD solutions isothermal cases. The following conclusions can be drawn from this study:

1. Increasing the $A_o/L$ ratio in small frequencies leads to more CO₂ transported to the right-hand side and outlet. After being transported through convection by the influence of the oscillation in the left-hand reservoir, the species tend to behave in
a diffusive way. Accumulation of CO₂ is found in the right-hand reservoir and outlet. This behavior is perfectly reasonable due to the molecular weight of this species compared to the lighter one as well as the difference in diffusion coefficient. The effect of the oscillatory wall is very significant when the high values of amplitudes and frequencies are assigned. A violent movement of the fluid is created in both left and right chambers resulting in fast forward and backward motions of the species. As a consequence of this effect, the CO₂ ratios are found to be very small and continuously decreasing in time. Also, from small to large $A_o/L$ ratios, the optimal points for every curve were obtained for increasing Womersley number increases. Those points represent the optimal frequencies and amplitudes in which CO₂ is transported from the left-hand reservoir to right-hand outlet under the influence of the oscillatory wall. In Conclusion, with small amplitudes larger frequencies need to be applied to achieve the optimal transport and separation in the system.

2. Regarding the Soret effect, it can be concluded, in general, that higher frequency and temperature, imply higher changes in the lighter species mass flow rate. Those results support the analytical theory developed by Ludwig (1856) and Soret (1856) [23]. Different behaviors of the species and changes in the tidal ratio of the concentrations were observed. For very high temperature changes, the Soret effect generates accumulation of species at the second reservoir. Even though CO₂ have larger molecular weight and diffusion coefficient than H₂ on a N₂ environment, the displacement and accumulation of the H₂ in the second reservoir is larger. That is also one of the most remarkable points; the thermal gradient induces a species transport with more influence than the effect of the convective term provided by the oscillating wall.
In figures 39 and 40 it can be seen how the lighter species reaches into the second tank with higher values of mass flow rate at extreme variations of temperature. Diffusion of the lighter species has the larger improvement.

Figure 39: CO\textsubscript{2} Concentration – T\textsubscript{cylinder} = 1000K

Figure 40: He Concentration – T\textsubscript{cylinder} = 1000K
On the other hand, small $\Delta T$ also drives the behavior, changes on the species concentration and the tidal ratio of the species concentration. The increment on the mass flow rate is found as temperature and frequencies increase.

3. Time accurate studies with user-defined functions and define-profile are very time consuming. The parallelization mode improves the computational efficiency in more than 100% in average. This statement is described in detail in Table 2.

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Table 2: Computational Time -Dynamic Mesh -FLUENT

Further studies may improve on the selection and behavior of boundary conditions. The inlet condition selected as 300K is the mean temperature at which the mixture reaches steady state before the oscillating wall and the Soret effect are imposed. In addition, creating a mechanism that contributes to keep homogeneous mixture inside of the reservoirs is also part of the actual research, as it can contribute to the species separation. Scaling laws and miniaturization of the model is part of the long term goal of this project.
APPENDIX A: FIGURES
Figure 41: Molar fraction of H₂ at f = 0.4 Hz

Figure 42: Molar fraction of CO₂ at f = 0.4 Hz
Figure 43: Molar fraction of H\textsubscript{2} at f = 0.5 Hz

Figure 44: Molar fraction of CO\textsubscript{2} at f = 0.5 Hz
Figure 45: Molar fraction of H$_2$ at $f = 0.6$ Hz

Figure 46: Molar fraction of CO$_2$ at $f = 0.6$ Hz
Figure 47: Molar fraction of CO2 at $f = 0.4$ Hz –Soret effect (Increasing Temperature)

Figure 48: Molar fraction of CO2 at $f = 0.5$ Hz –Soret effect (Increasing Temperature)
Figure 49: Molar fraction of CO2 at f = 0.6 Hz – Soret effect (Increasing Temperature)

Figure 50: Molar fraction of CO2 at f = 0.4 Hz – Soret effect (Decreasing Temperature)
Figure 51: Molar fraction of CO2 at f = 0.5 Hz – Soret effect (Decreasing Temperature)

Figure 52: Molar fraction of CO2 at f = 0.6 Hz – Soret effect (Decreasing Temperature)
Figure 53: Molar fraction of H$_e$ at $f = 0.4$ Hz –Soret effect (Increasing Temperature)

Figure 54: Molar fraction of H$_e$ at $f = 0.5$ Hz –Soret effect (Increasing Temperature)
Figure 55: Molar fraction of $H_e$ at $f = 0.6$ Hz – Soret effect (Increasing Temperature)

Figure 56: Molar fraction of $H_e$ at $f = 0.4$ Hz – Soret effect (Decreasing Temperature)
Figure 57: Molar fraction of $H_e$ at $f = 0.5$ Hz – Soret effect (Decreasing Temperature)

Figure 58: Molar fraction of $H_e$ at $f = 0.6$ Hz – Soret effect (Decreasing Temperature)
Figure 59: Molar fraction of H$_2$ at f = 0.5 Hz – Soret effect (T=200K)

Figure 60: Molar fraction of CO2 at f = 0.4 Hz – Soret effect (T=200K)
APPENDIX B: TABLES
#!/bin/sh

# prepare a UDF library for parallel use
# usage: pudf [hostpfx]

h=${1:-1}
shift
if [ "$h" = "" ] ; then
  hosts=$HOME/hosts.fluent
else
  hosts=$HOME/$h.hosts.fluent
fi

echo host from $hosts

scriptfile=$HOME/bin/compile-udf-jou
if [ ! -d $HOME/bin ] ; then
  mkdir $HOME/bin
fi
if [ ! -f $scriptfile ] ; then
  cat <<EOF > $scriptfile
  (cx-gui-do cx-activate-item "MenuBar*FunctionsSubMenu*Compiled...")
  (cx-gui-do cx-activate-item "Compiled UDFs*Table1*Frame1*PushButton2( Add)"
  (cx-gui-do cx-set-text-entry "Select File*FilterText" ".c")
  (cx-gui-do cx-activate-item "Select File*Apply"
  (cx-gui-do cx-add-list-items "Select File*Frame14*Frame1*Frame1*List1" "piston_modified_2.c") #f)
  (cx-gui-do cx-activate-item "Select File*OK"
  (cx-gui-do cx-activate-item "Compiled UDFs*PushButton3(Build)"
  (cx-gui-do cx-activate-item "Warning*OK"
  (cx-gui-do cx-activate-item "Compiled UDFs*Table1*Frame1*PushButton2( Add)"
  (cx-gui-do cx-set-text-entry "Select File*FilterText" ".c")
  (cx-gui-do cx-activate-item "Select File*Apply"
  (cx-gui-do cx-add-list-items "Select File*Frame14*Frame1*Frame1*List1" "temperature.c") #f)
  (cx-gui-do cx-activate-item "Select File*OK"
  (cx-gui-do cx-activate-item "Compiled UDFs*PushButton3(Build)"
  (cx-gui-do cx-activate-item "Warning*OK"
  (cx-gui-do cx-activate-item "Compiled UDFs*PanelButtons*PushButton1(Cancel)"
  (cx-gui-do cx-activate-item "MenuBar*FileMenu*Exit")
  EOF
  echo creating script file using filename piston_modified_2.c
fi

echo host from $hosts
if [ ! -f $hosts ] ; then
  echo no host file $hosts
  exit 1
fi

fluent -t0 -pnmpi 3d -i $scriptfile

if [ ! -d libudf ] ; then
  echo No UDF library
  exit 1
fi
dir=`pwd`
for i in `sort -u $hosts` ; do
  echo " distributing to $i"
  rsh $i "mkdir -p $dir"
  rsync -e rsh -a libudf $i:$dir/
done

Table 3: Parallelization - UDF – Define Profile Code - Cluster
p=${1:-7}
h=${2:-1}
shift
shift
parallel $p
host from /home/jalmiron/$h.hosts.fluent
if [ ! -f /home/jalmiron/$h.hosts.fluent ] ; then
echo no host file /home/jalmiron/$h.hosts.fluent
exit 1
fi
fluent -t$p -pnmpi -cnf=/home/jalmiron/$h.hosts.fluent 3d "$@"

Table 4: Parallelization Code – Cluster - FLUENT

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Table 5: Womersley Number – Tidal Ratio of Species for 5%, 7%, and 10% - UCF

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Table 6: Womersley Number – Tidal Ratio of Species for 5%, 7%, and 10% - UF
LIST OF REFERENCES


[9] Bowden, K. F., “Horizontal mixing in the sea due to a shearing Current,” Journal of Fluid Mechanics, Number 21, 83 to 95


