

# The Physics of Detonation Chemistry: A Radical Theory in Predicting the Deflagration to Detonation Transition and Environmental Explosions

V.R. Sanal Kumar (✉ [vr\\_sanalkumar@yahoo.co.in](mailto:vr_sanalkumar@yahoo.co.in))

Indian Space Research Organisation

**Nichith Chandrasekaran**

Indian Institute of Science Bangalore

**Vigneshwaran Sankar**

Indian Institute of Technology Kanpur

**Ajith Sukumaran**

Kumaraguru College of Technology, Coimbatore

**Sivabalan Mani**

Georgia Institute of Technology

**Tharikaa Ramesh kumar**

Auburn University

**Sathyan Padmanabhan**

University of Arizona

**Vignesh Saravanan**

Seoul National University

**Vishnu Natarajan**

Pusan National University

**Hema Sai Nagaraju Doddi**

Embry–Riddle Aeronautical University

**Mohammed Niyasdeen Nejaamtheen**

King Fahd University of Petroleum and Minerals

**Sulthan Ariff Rahman Mohamed Rafic**

Kumaraguru College of Technology, Coimbatore

**Roshan Vignesh Baskaran**

Kumaraguru College of Technology, Coimbatore

**Pavithra Murugesh**

Kumaraguru College of Technology, Coimbatore

**Amrith Mariappan**

Kumaraguru College of Technology, Coimbatore

**Thianesh U.K**

Kumaraguru College of Technology, Coimbatore

**Anand moorthi**

Kumaraguru College of Technology, Coimbatore

**Mohan Elumalai**

Kumaraguru College of Technology, Coimbatore

**Pradeep Kumar Pavalavanni**

GITAM University

**Rajaghatta Sundararam Bharath**

Indian Institute of Science Bangalore

**Charlie Oommen**

Indian Institute of Science Bangalore

**Pradeep Kumar Radhakrishnan**

Pusan National University

**Shiv Kumar Choudhary**

All India Institute of Medical Sciences

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**Research Article**

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# **The Physics of Detonation Chemistry: A Radical Theory in Predicting the Deflagration to Detonation Transition and Environmental Explosions**

**Running Title: Environmental and Supernova Explosions – A New Perspective**

V.R.Sanal Kumar<sup>\*,a,b,c</sup>, Nichith Chandrasekaran<sup>b,c</sup>, Vigneshwaran Sankar<sup>b,c,k</sup>, Ajith Sukumaran<sup>c,d</sup>, Sivabalan Mani<sup>c,e</sup>, Tharikaa Ramesh kumar<sup>c,f</sup>, Sathyan Padmanabhan<sup>c,g</sup>, Vignesh Saravanan<sup>c,d</sup>, Vishnu Natarajan<sup>c,h</sup>, Hema Sai Nagaraju Doddi<sup>c,i</sup>, Mohammed Niyasdeen Nejaamtheen<sup>c,j</sup>, Sulthan Ariff Rahman Mohamed Rafic<sup>c</sup>, Roshan Vignesh Baskaran<sup>c</sup>, Pavithra Murugesh<sup>c</sup>, Amrith Mariappan<sup>c</sup>, Thianesh U.K<sup>c</sup>, Anand moorthi<sup>c</sup>, Mohan Elumalai<sup>c</sup>, Pradeep Kumar Pavalavanni<sup>c,h</sup>, Rajaghatta Sundararam Bharath<sup>b</sup>, Charlie Oommen<sup>b</sup>, Pradeep Kumar Radhakrishnan<sup>l,m</sup>, Shiv Kumar Choudhary<sup>m</sup>

<sup>a</sup> Indian Space Research Organisation, VSSC, Trivandrum 695 022, Kerala, India

<sup>b</sup> Indian Institute of Science, Bangalore 560 012, India

<sup>c</sup> Kumaraguru College of Technology, Coimbatore 641 049, Tamil Nadu, India

<sup>d</sup> Seoul National University, Gwanak-gu, Seoul 08826, Republic of Korea

<sup>e</sup> Georgia Institute of Technology, Atlanta, GA 30332-0150, U.S.A

<sup>f</sup> Auburn University, Auburn, AL 36849-5338, U.S.A

<sup>g</sup> The University of Arizona, Tucson, AZ 85721, U.S.A

<sup>h</sup> Pusan National University, Geumjeong-gu, Busan 46241, Republic of Korea

<sup>i</sup> Embry-Riddle Aeronautical University, Daytona Beach, FL 32114-3900, U.S.A

<sup>j</sup> King Fahd University of Petroleum and Minerals, Dahran – 31261, Kingdom of Saudi Arabia

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\*Corresponding Author, Professor and Aerospace Scientist (ISRO – SC CA 6301/2013), and Project coordinator of Indo-Russian Project at IISc, Senior AIAA Member and Member, American Heart Association; vr\_sanalkumar@yahoo.co.in; +91-8754200501

<sup>k</sup> Indian Institute of Technology, Kanpur, India

<sup>l</sup> GITAM University, Visakhapatnam, India

<sup>m</sup> All India Institute of Medical Sciences, New Delhi, India

**\*Corresponding Author :** Prof.V.R.Sanal Kumar, *Email:* vr\_sanalkumar@yahoo.co.in

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## Abstract

The theoretical finding of the *Sanal-flow-choking* [**PMCID: PMC7267099**] and streamtube flow choking (*V.R.Sanal Kumar et al., Physics of Fluids, Vol.33, No.3, 2021, DOI: 10.1063/5.0040440*) are methodological advancements in predicting the *deflagration-to-detonation-transition* (DDT) in the real-world-fluid flows (continuum/non-continuum) with credibility.<sup>[1,2]</sup> Herein, we provide a proof of the concept of the *Sanal-flow-choking* and *streamtube-flow-choking* causing DDT in wall-bounded and free-external flows. Once the streamlines compacted, the considerable pressure difference attains inside the streamtube and the flow gets accelerated to the constricted region for satisfying the continuity condition set by the conservation law of nature. If the shape of the streamtube in the internal/external flow is similar to the convergent-divergent (CD) duct the phenomenon of the *Sanal-flow-choking* and supersonic flow development occurs at a critical-total-to-static pressure ratio (CPR) in *yocto* to *yotta* scale systems and beyond, which leads to shock wave generation or detonation as the case may be. At the lower critical detonation or hemorrhage index, the CPR of the reacting flow and the critical blood-pressure-ratio (BPR) of the subjects (human being/animal) are unique functions of the heat-capacity-ratio (HCR) of the evolved gas in the CD duct (*V.R.Sanal Kumar et al., Global Challenges, Wiley Publication, January 2021, DOI: 10.1002/gch2.202000076, PMCID: PMC7933821*; Sanal Kumar V.R et al. Stroke, Vol.

52, Issue Suppl\_11 March 2021, doi.org/10.1161/str.52.suppl\_1.P804). In silico results are presented herein to establish the proof of the concept of the *Sanal-flow-choking* and *streamtube-flow-choking* causing shock-wave/detonation in diabatic flow systems and *asymptomatic-hemorrhagic-stroke* in biological systems. The physics of detonation chemistry presented herein sheds light for exploring environmental and supernova explosions.<sup>[107]</sup> *In silico* results reported herein provide an authentic answer to many unresolved research questions in Physics in general and aerospace, mechanical, biological, chemical, energy, environmental, nano and material sciences in particular.

**Key words:** Deflagration-to-detonation-transition (DDT), Detonation, Nanofluid flow system design, *Hemorrhagic-stroke*, Sanal flow choking, *Streamtube-flow-choking*, Chemical Rocket, Environmental and Supernova Explosions.

## Introduction

Although the underlying knowledge in advanced science of real-world flows (continuum / non-continuum) with the multi-disciplinary focus has been evolved over the centuries there are still many unresolved problems due to the lack of fundamental understanding of physics and chemistry of diabatic fluid flows (flow involves transfer of heat) in chemical energy systems.<sup>[1]</sup> Such problems of urgency to the scientific communities are the prediction and attenuation of detonation in reacting fluid flow systems and that of *asymptomatic stroke* (AS) in the human circulatory system (HCS). Note that the *deflagration to detonation transition* (DDT) in reacting fluid flow systems and the creeping flow to *asymptomatic hemorrhagic stroke* (AHS) in biological systems could happen due to the consequence of the Sanal flow choking<sup>[1-9]</sup> <<https://pubmed.ncbi.nlm.nih.gov/32837737/>>. Over the decades several *in vitro* and *in silico* studies were reported on DDT in various chemical energy systems from *yocto* to *yotta* scales but

there were no authentic answers on the fundamental cause of DDT in real-world fluid flow systems.<sup>[10-20]</sup> Modeling and simulation of *nanoscale* fluid flow is truly intricate, because in the contrary to *milli-scale* or *macroscale* fluid flow, the governing-equations capturing exact flow physics and chemistry are not well delineated.<sup>[21-26]</sup> Hence, even if the *in silico* method is well suited for the solution of considered problem, *in vitro* methods in *nanoscale* are having inherent inaccuracy for generating benchmark data for *in silico* code verification. Therefore, one should rely up on the exact solution for generating benchmark data for solving unresolved problems carried forward over the centuries with credibility. Such models should scrupulously satisfy the conservation laws as imposed by our nature. Therefore, the *Sanal flow choking* models<sup>[1]</sup> should be invoked for *in silico* model validation, verification and calibration before featuring fluid flow characteristics of *yocto* to *yotta* scale diabatic fluid flow systems and beyond with reliability.

Of late, small scale systems have got significant attention in the industry because mostly micro/nano-electromechanical systems (MEMS/NEMS) are based on the fluid motion.<sup>[21]</sup> This is particularly true in the *nano medicine* for drug discovery and nano/micro thrusters for aerospace systems design. Obviously, the *nano scale* fluid flow system development in microgravity aerospace application is a challenging research topic. Furthermore, such systems in atmospheric conditions applicable to physical, chemical, and biological sciences are also challenging areas for research due to the pragmatic difficulties to perform *in vitro* and *in silico* studies and in addition the lack of closed-form analytical models for benchmarking. Various researchers reported through *in vitro* and *molecular dynamics* simulations that the surface friction compared to the fluid flow is very low for *carbon nanotubes* (CNT).<sup>[26-29]</sup> The fact is that the reported results were not supported with benchmark data generated from any exact solution for meeting all the conservation laws of nature.

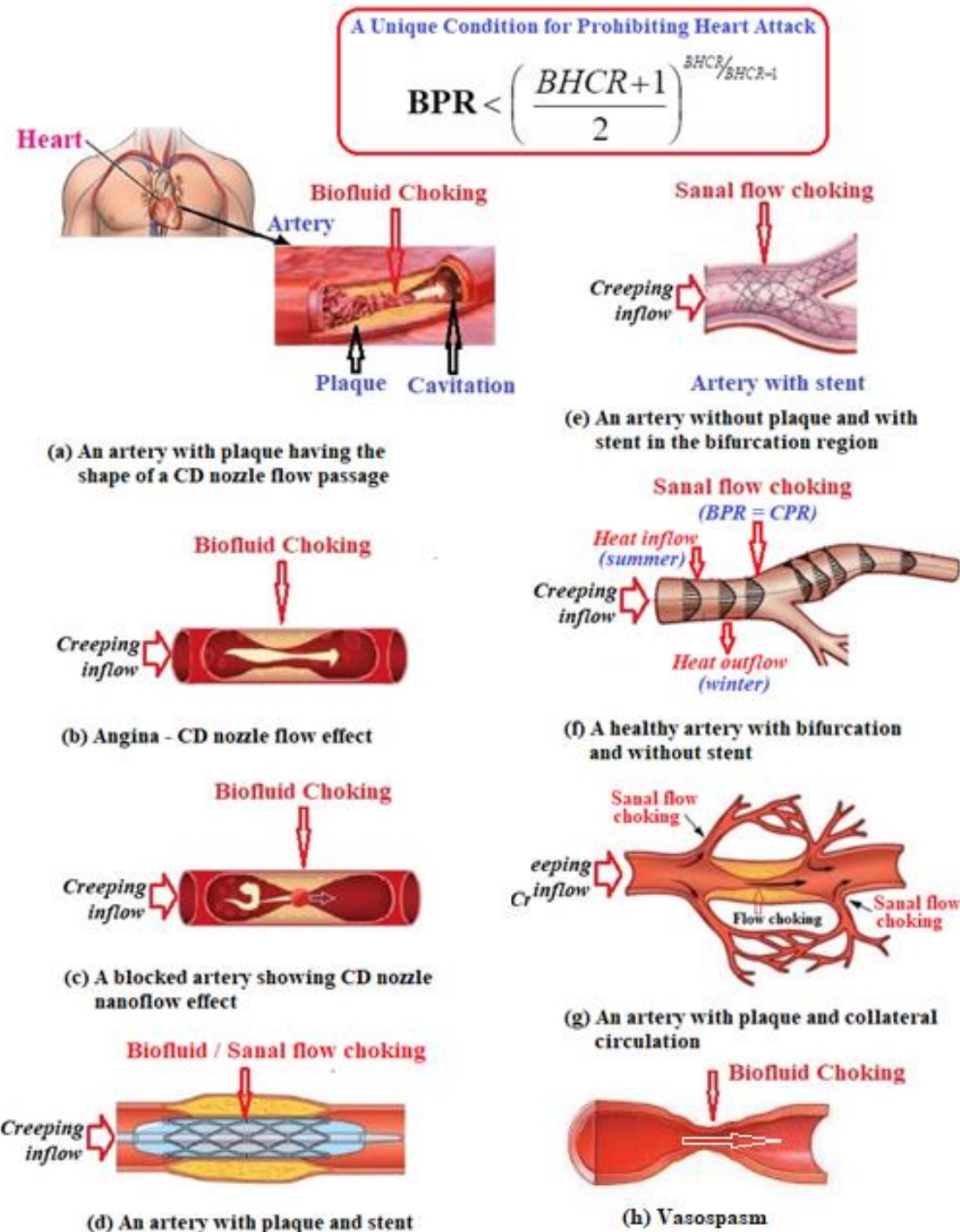
Qi-Long Yan et al.<sup>[30]</sup> reported (2016) that encapsulation of energetic molecules into CNTs is extremely challenging and still demanding additional analytical and *in vitro* studies to understand its sensitivity and performances<sup>[31-34]</sup> having with highly sensitive energetic material (EMs). Gunpowder, a firearm propellant, invented in ancient China is believed as the earliest energetic material,<sup>[30]</sup> which generally does not detonate but rather deflagrates. The deflagration and detonation properties of black powder however differ significantly from new generation high energetic solid propellants<sup>[35, 36]</sup> and there are no authentic predictive models available as on the date to forecast these properties at nanoscale. Therefore, *in silico* simulation of DDT in the real-world nanofluid flow system is the need of the 21st century; and it must be verified with an exact solution for a credible decision making.<sup>[36-38]</sup> Admittedly, there are no literature available on *in silico* simulation of DDT in milli-scale or nanoscale systems having port with the sudden expansion/divergence region.<sup>[39-45]</sup>

The Sanal flow choking, a compressible fluid flow effect, is a radical theory in advanced science of real-world fluid flow systems,<sup>[1]</sup> which is capable to provide solutions to many unanswered research questions in the continuum and non-continuum fluid flows moved ahead over the centuries.<sup>[46-62]</sup> Note that the non-continuum or nanoscale fluid flows obey all conservation laws of nature. Indeed, all fluids available in our nature are compressible.<sup>[1]</sup> In the case of nanoscale fluid flows, when pressure increases the *Knudsen number* reduces causing the compressible viscous flow effect due to the decrease in the average mean free path heading to zero-slip wall boundary condition. All these deliberations corroborate that the *Sanal flow choking* model puts a focal role in interdisciplinary science for performing *in-silico* experiments with credibility in the continuum and non-continuum fluid flows in *yocto* to *yotta* scale systems. Certainly, at the *Sanal flow choking* condition for diabatic flows (flow involves transfer of heat)

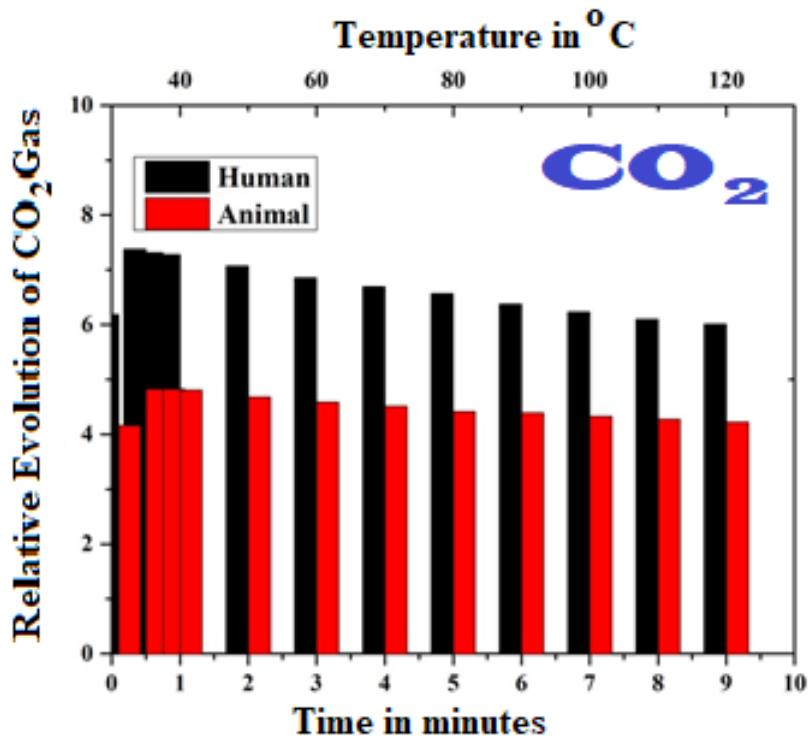
all conservation laws of nature are contented. Any fluid flow solver calibrated with the *Sanal flow choking* condition of diabatic flow could be capable to predict *a priori* the risk of DDT in chemical energy systems and AHS in biological systems.<sup>[1]</sup> It could be achieved by predicting the lower critical detonation index (LCDI) and the lower critical hemorrhage index (LCHI) as the case may be. It is pertinent to note that both the LCDI and the LCHI are representing the critical pressure ratio of the respective systems. These indexes are regulated by the *heat-capacity-ratio* (HCR) of the evolved gas with the lowest HCR <DOI: 10.1002/gch2.202000076>.

In this article we are primarily focusing on analytical modeling and *in silico* simulation of a diabatic fluid flow system aiming to demonstrate the *Sanal flow choking*, *streamtube flow choking*, shock wave generation and pressure overshoot for proving the concept of the occurrence of DDT in a classical straight-tube ending with a divergent port geometry at the subsonic inflow condition. This physical situation is analogous to the creeping flow to the choked flow condition in an artery with the divergent/bifurcation/vasospasam region causing AHS (see Figure 1(a-h) as the central illustration).<sup>8</sup> Herein, we made an effort to correlate the radical theory of the *Sanal flow choking* in the human circulatory system (HCS) because blood is a compressible fluid.<sup>[1]</sup> Furthermore, *in vitro* study shows (see Fig.2) that carbon dioxide (CO<sub>2</sub>) gas is predominant in fresh-blood samples of the healthy human-being than *Guinea-pig* at a temperature range of 37-40<sup>0</sup> C (98.6-104<sup>0</sup> F), which increases the risk of flow-choking leading to AHS. It is an admitted fact that the *Sanal flow choking* steers to the shock-wave generation in viscoelastic tubes with vasospasm (see the attached *in vitro* results as **movie S1** and **S2**) like blood vessels, which create memory effect leading to AHS in the later stage. Herein, we are focusing our research contents for chemical and environmental science system designers with original and novel fundamental research and

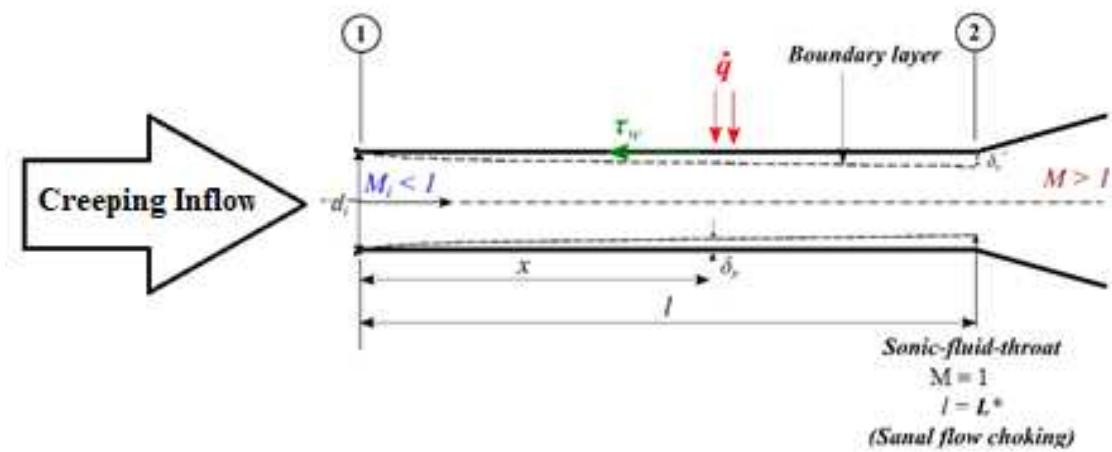
discussion of new developments in chemical engineering, which illustrates the transfer of techniques from biological sciences.



**Figure 1(a-h).** Internal flow choking in HCS (The Central Illustration) [1]



**Figure 2.** *In vitro* result shows the mass spectrum of carbon dioxide (CO<sub>2</sub>) evolved as a function of both time and temperature in blood samples of healthy subjects at 37-40° C (98.6-104° F) and beyond the physiological range (the human being / *Guinea-pig*) [5].



**Figure 3.** Demonstrating the *Sonal flow* choking condition in an internal fluid flow system.

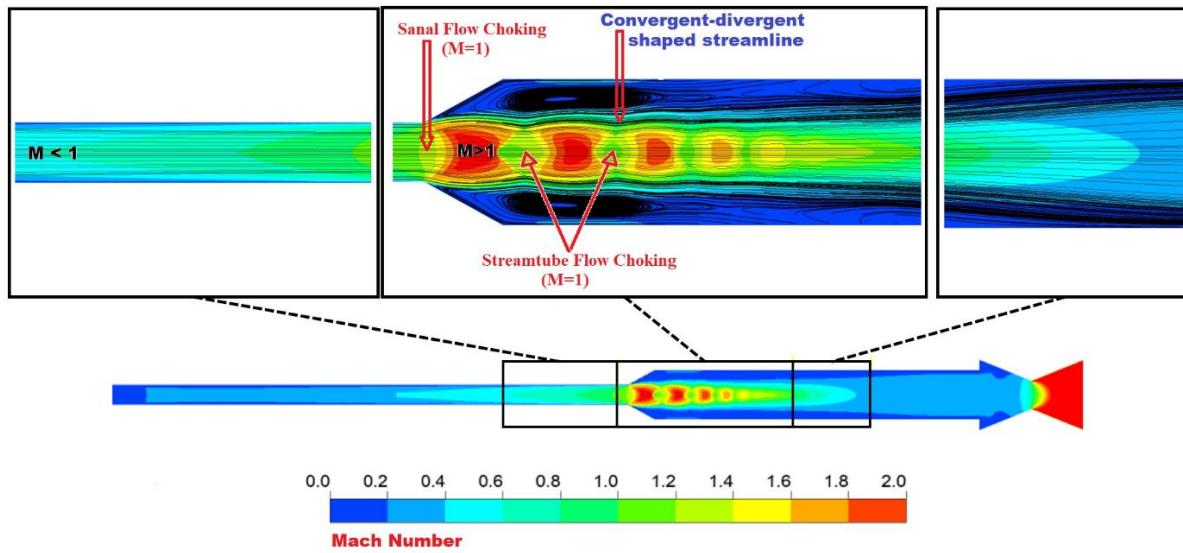
Over the decades many blood flow simulation studies have been carried out with the incompressible fluid flow assumption [63-78], which are useful only for simulating the creeping flow conditions in the human circulatory system (HCS). Herein, we established the proof of the concept of DDT and AHS at the creeping inflow condition in an internal diabatic flow system (see **Figure 3**) through *in silico* modeling at a critical total-to-static pressure ratio (CPR) where the compressibility effect is significant. The importance of this interdisciplinary study design is succinctly reviewed in the subsequent background section for highlighting the research question pertaining to an authentic prediction of LCDI and LCHI.

## Background

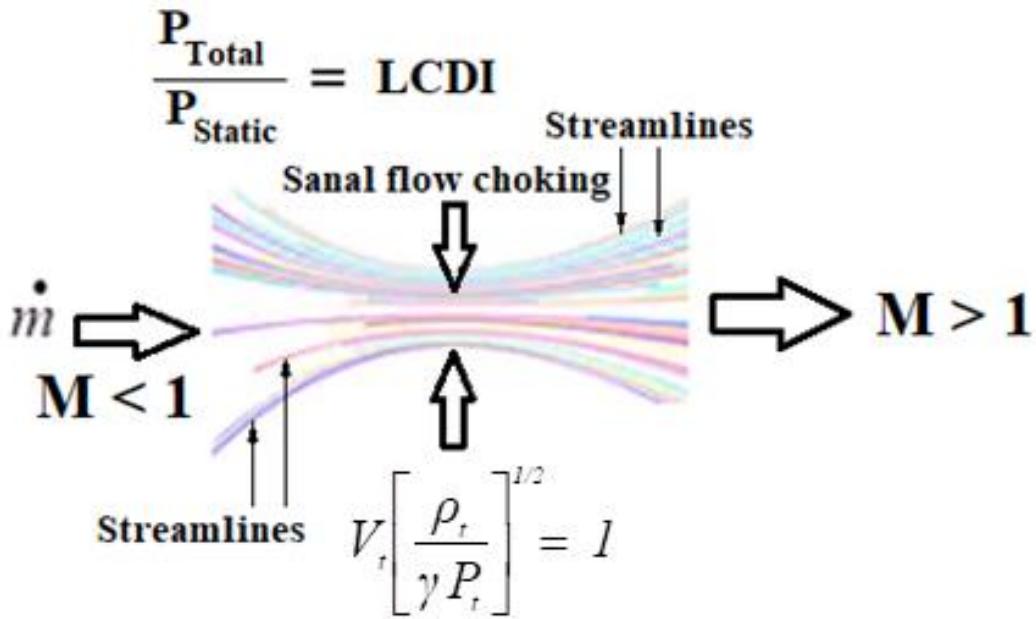
Of late many *in silico* studies have been reported in base fluids and nanofluids for various industrial applications without an authentic validation of the results with benchmark data. As the pressure of the *nanofluid* rises, *average-mean-free-path* diminishes and thus, the *Knudsen number* lowers heading to a zero-slip wall-boundary condition with compressible viscous (CV) flow regime.<sup>[2]</sup> V.R.S.Kumar et al.<sup>[1-3]</sup> presented an exact analytical solution, which is capable to predict precisely the three-dimensional boundary-layer blockage factor (*named herein as blockage factor*) of diabatic fluid flow systems at the zero-slip-length. The innovation of the *Sanal flow choking* model was established through the entropy relation, as it meets all the conservation laws of nature.<sup>[1]</sup> The physical insight of the *Sanal flow choking* and *streamtube* flow choking demonstrated herein sheds light on getting answers of several unanswered research questions in chemical and advanced sciences.

V.R.S.Kumar et al.<sup>[1-9]</sup> established that there are likelihoods of Sanal flow choking in HCS (see **Figure 1(a-h) as the central illustration**), after attaining the critical blood pressure ratio.<sup>[1,7]</sup> The experiences gained from the theoretical and *in vitro* findings (see **Figure 2**) prompted us for the

internal flow simulation of the straight duct ending with a divergent port for examining *Sanal flow choking* and streamtube flow choking (see **Figure 3** and **Figure 4(a-b)**) through the reliable *in silico* simulation. It is a well-recognized fact that, the entire governing equations for viscous flows are extremely challenging to solve analytically using the existing mathematical tools. Using the developing system of non-linear equations, the *in silico* simulation with multi-phase and multi-species composite fluid flow with oscillating boundary wall is also a challenging task. It is because of the fact that an accurate, strong and competent solution with the super fine grid system is critical for the high reliability *in silico* modelling.<sup>[1-3]</sup>



**Figure 4(a).** The enlarged view of the *Sanal flow choking* and the streamtube flow choking phenomena in an idealized physical model of an internal fluid flow system <Movie: <https://youtu.be/bv3ZDcPKMSI>>.



**Figure 4(b).** Demonstrating the CD duct flow effect in *yocto* to *yotta* scale

internal and external flow systems leading to streamtube flow choking.

Physics of *Sanal flow-choking* received significant attention in the global scientific community for solving various research problems of topical interest.<sup>[1,2,7,8]</sup> Certainly, using the *Sanal flow choking* model to predict the 3D blockage factor, the chemical rocket motor designer could optimize the grain port geometry with the maximum possible propellant loading density with the allied igniter, without inviting DDT and without any costly empirical design technique or *in silico* simulation.<sup>[2]</sup> Of late (2020) V.R.S.Kumar et al.<sup>[2]</sup> highlighted the physical significance of the detonation kernel associated with the 3D blockage factor and the critical pressure ratio (CPR) causing the phenomenon of Sanal flow choking in a constant area duct ending with a divergent port. Through this study,<sup>[2]</sup> the fundamental cause of DDT in the chemical rocket has come to the foreground. Over the centuries the scientific communities under the strong impression that at the creeping inflow condition DDT won't occur in a straight duct ending with a divergent region. We

could authentically disprove this wrong notion on DDT through a closed-form analytical model, *in silico* results<sup>[3]</sup> and the full motor static test results.<sup>[1]</sup> Thereby, a popular research question revolving through the globe over the centuries has been settled with a cogent answer. In brevity, it says that due to the *Sanal flow choking* the creeping or low subsonic flow (continuum or non-continuum) will get augmented to the supersonic flow condition in a straight duct ending with a divergent port and create possible shock waves and shock diamonds due to streamtube flow choking (see **Figure 4 (a-b)**). Note that the *Sanal flow choking* and the *streamtube* flow choking are new theoretical concepts applicable to both the continuum and non-continuum fluid flows. Once the streamlines compacted, the considerable pressure difference attains within the streamtube and the flow within the streamtube gets enhanced to the constricted section for satisfying the continuity condition set by the conservation law of nature, which leads to the *Sanal flow choking* and supersonic flow development at a CPR due to the convergent-divergent (CD) shape of the streamtube (see Figure 4(a-b)). For authenticating the proof of the concept the analytical and *in silico* methodologies are presented in the subsequent section.

## Methodology

Analytical and *in silico* methodologies are invoked herein for establishing the proof of the concept of the occurrence of DDT and AHS at the creeping inflow condition in a constant area duct ending with a divergence/bifurcation region (see Figure 3). **Figure 3** is highlighting the *Sanal flow* choking condition in such a classical model of a real-world fluid flow system and **Figure 4(a)** is depicting the *Sanal flow* choking and streamtube flow choking corresponding to **Figure 3**. **Figure 4(b)** shows the enlarged view of streamline pattern and the streamtube flow choking in *yocto* to *yotta* scale internal and external flow systems. It is highlighting the CD duct flow effect in a streamtube leading to detonation in the chemical energy and environmental systems at a CPR.

Physical situations of flow choking depicted in **Figure 3** and **Figure 4(a-b)** are meeting the conditions set by the conservation laws of nature. This is a remarkable finding for solving various unresolved problems in aerospace, biomedical, chemical, environmental, material, mechanical and nanotechnology, oil and natural gas industries.<sup>[1]</sup>

At the unchoked flow condition pressure in the constricted region of the streamtube will be lower than the wider region and this physical situation leads to choked flow condition at the CPR. Note that CPR is governed by HCR. When the streamtube is compressed, the reduction in internal energy is transformed into an accelerated fluid flow motion to satisfy the law of conservation of mass, which leads to the *Sanal flow choking* in CD shaped streamtube heading to the generation of supersonic flow causing shock waves, pressure-overshoot and detonation in the downstream region of the *streamtube*. These analytical findings are corroborated with the *in silico* results presented in the subsequent section.

The *fluid-throat* induced internal flow choking in real-world fluid flow systems at the creeping inflow condition is a new concept, which is defined as *Sanal flow choking*,<sup>[1]</sup> a phenomenon occurs due to the boundary layer blockage.<sup>[1-9]</sup> The exact solution of the 3D boundary layer blockage (BLB), corresponding to LCDI (i.e., considering the lowest value of HCR ( $\gamma_{\text{lowest}}$ ) of the evolved gases), at the Sanal flow choking for diabatic flows (continuum / non-continuum) with respect to **Figure 3** is given in Equation 1.  $M_i$  is the subsonic upstream inflow Mach number. **Figure 5** is the solution curve of BLB for both 2D<sup>[4]</sup> and 3D cases (Equation 1). Note that irrespective of the magnitude of the BLB factor, the *Sanal flow choking* occurs anywhere in the circulatory circuit once the flow attains the critical pressure ratio (see Figure 5). The critical pressure ratio is dictated by the heat capacity ratio (HCR or  $\gamma$ ) of the evolved gas with the lowest HCR (see Equation 2 and 3). Note that BLB will never be zero in any real-world fluid flow system.<sup>[1, 82]</sup> Equation 2 represents

the LCDI, which is estimated based on the  $\gamma_{\text{lowest}}$  for attaining the *Sanal flow choking* condition. Equation 2 reveals that in any flow system, the total-to-static pressure ratio ( $P_{\text{total}}/P_{\text{static}}$ ), should at all times be lesser than the LCDI for negating the undesirable detonation. In the case of biological flows Equation 2 is re-cast with respect to the blood pressure ratio (BPR) and the blood/biofluid heat capacity ratio (BHCR) for estimating the LCHI, which is presented herein as Equation 3. It is evident from Equation 3 that for negating AHS, the BPR should maintain always lesser than LCHI, which is governed by the lowest HCR of the evolved gas in the vessel. In the HCS the total pressure indicates the *systolic blood pressure* (SBP) and the static pressure shows the *diastolic blood pressure* (DBP).

$$BLB|_{@M_{xz}=1} = \left[ 1 - M_i^{1/2} \left[ \frac{2}{\gamma_{\text{lowest}} + 1} \left( 1 + \frac{\gamma_{\text{lowest}} - 1}{2} M_i^2 \right) \right]^{\frac{\gamma_{\text{lowest}} + 1}{4(1 - \gamma_{\text{lowest}})}} \right] d_i \quad (1)$$

$$\left( \frac{P_{\text{total}}}{P_{\text{static}}} \right)_{\text{fluid throat}} < LCDI = \left( \frac{\gamma_{\text{evolved gases with the lowest } \gamma} + 1}{2} \right)^{\frac{\gamma_{\text{lowest}}}{\gamma_{\text{lowest}} - 1}} \quad (2)$$

$$\frac{SBP}{DBP} = BPR < LCHI = \left( \frac{BHCR + 1}{2} \right)^{\frac{BHCR}{BHCR - 1}} \quad (3)$$

$$M_i = \frac{1}{\gamma_{\text{lowest}}^{1/2}} \left[ (\gamma_{\text{lowest}} + 1) \left( \frac{2}{\gamma_{\text{lowest}} + 1} \right)^{\frac{\gamma_{\text{lowest}}}{\gamma_{\text{lowest}} - 1}} - 1 \right]^{1/2} \quad (4)$$

$$\bar{f} = \frac{d_i}{4L^*} \left[ \frac{1 - M_i^2}{\gamma_{\text{lowest}} M_i^2} + \frac{\gamma_{\text{lowest}} + 1}{2\gamma_{\text{lowest}}} \ln \left[ \frac{(\gamma_{\text{lowest}} + 1)M_i^2}{2 + (\gamma_{\text{lowest}} - 1)M_i^2} \right] \right] \quad (5)$$

$$Mach\ number \ < \ 1 \quad (6)$$

$$\frac{Mass\ flow\ rate}{Port\ crossectional\ area} \left[ \frac{C_v\ (Diffusivity)}{P_x\ static\ (Conductivity)} \right]^{1/2} \ < \ 1 \quad (6a)$$

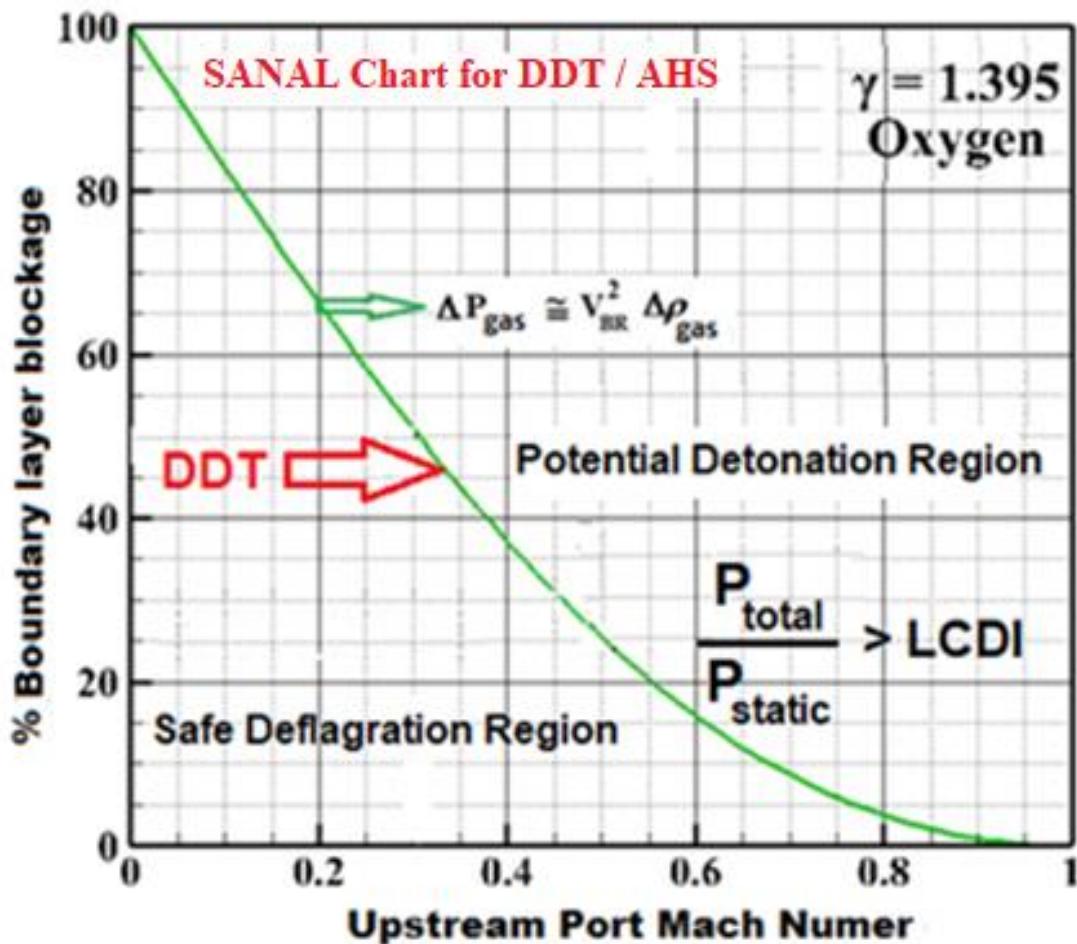
$$Biofluid\ Flow\ Velocity \left[ \frac{Blood\ Density}{(Heat\ Capacity\ Ratio)(Diastolic\ Blood\ Pressure)} \right]^{1/2} \ < \ 1 \quad (6b)$$

$$\left[ \frac{(Biofluid\ Flow\ Rate)_{local}\ (Blood\ Viscosity)_{local}}{(BHCR)_{lowest}\ (DBP)\ (Vessel\ Cross - sectional\ Area)_{local}} \right]^{1/2} \ < \ 1 \quad (6c)$$

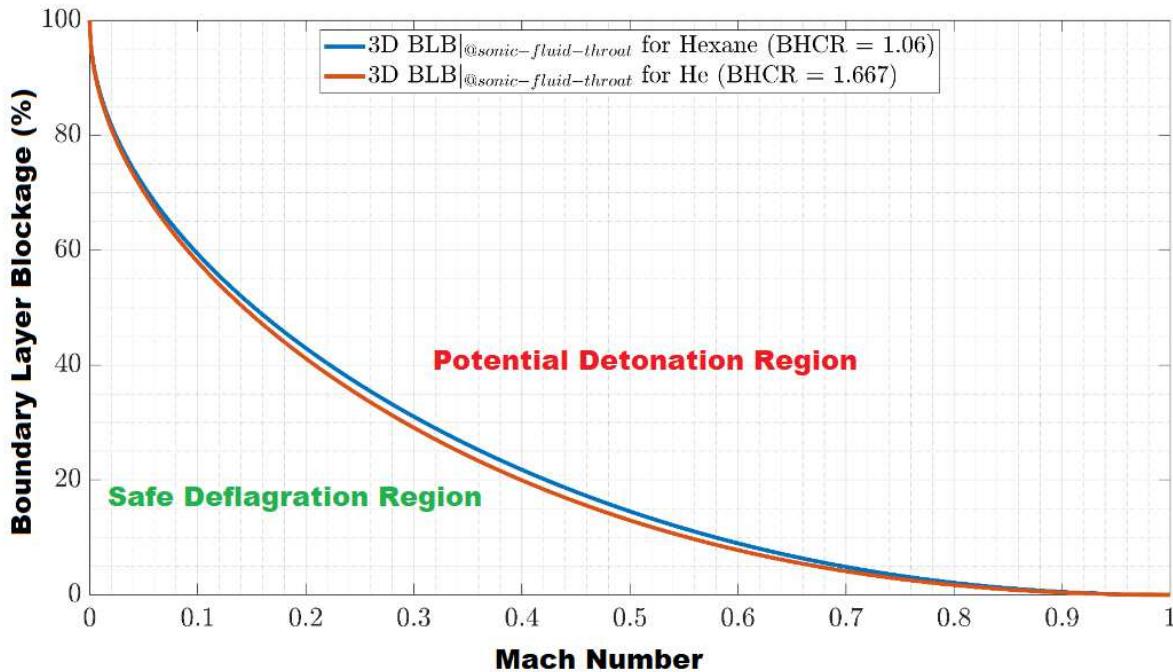
$$\frac{(Reynolds\ Number)(Kinematic\ Viscosity)}{Hydraulic\ Diameter} \left[ \frac{Blood\ Density}{(BHCR)\ (DBP)} \right]^{1/2} \ < \ 1 \quad (6d)$$

Equation 4 shows the inlet Mach number estimation for getting diabatic flow choking in a straight duct.<sup>[1]</sup> Equation 5 is a remarkable closed-form analytical model capable to predict the average friction coefficient,  $\bar{f}$  of any wall-bounded flow system, without any empiricism, for an authentic *in silico* simulation.<sup>[3]</sup> If we know  $\bar{f}$  and the length-to-diameter ( $l/d_i$ ) ratio we could fix the inflow Mach number for prohibiting DDT. Equation 5 will enable us for getting a choked flow condition at station 2 (see Figure 3) for the calibration of various *in silico* flow solvers by matching the numerically predicted blockage factor and the exact analytical solution.

The *Sanal* flow choking and streamtube flow choking are regulated by the physical situations set by Equations 1-6. It is a well known fact that for negating the flow choking Mach number should always be less than one in the system (see Equation 6). Equations 6(a-d) are the corollary of Equation 6. The self-explanatory Equations 6(a-d) derived from the compressible flow theory<sup>[1,4, 83]</sup> are representing Mach number, which are complimenting with Equation 2 and Equation 3. All



**Figure 5 (a).** Demonstrating the condition of DDT and AHS in an internal flow system at the Sanal flow choking condition (2D case).



**Figure 5 (b).** Demonstrating the condition of DDT in an internal flow system at the Sanal flow choking condition for two different gases (3D case).

these equations set the conditions for prohibiting *Sanal flow choking* and streamtube flow choking in any real-world fluid flow system. The individual or coupled effects of vessel geometry (stenosis) and the thermo-physical properties on flow choking can be easily discerned from Equations 6(a-d). These equations (Equations 6(a-d)) are well correlated with the clinical findings.<sup>[5-8]</sup> It is evident from Equation 6(a,c,d) that an increase in blockage factor (*i.e.*, a decrease in the port-cross-sectional-area), in any vessel due to plaque and/or boundary layer induced blockage, could increase the risk of *Sanal flow choking* in the creeping inflow condition. As directly evidenced from Equations 2, 3 and 6(b-d), the risk of *Sanal flow choking* could be negated by increasing the HCR of the evolved gas in the vessel. Note that the left hand side of Equations 6(a-d) are representing the magnitude of Mach number, which could be estimated from the biofluid properties and the vessel port area for estimating the risk of internal flow choking (see Figure 5).

It is important to note that the flow Mach number must always be less than one in the circulatory circuit including the *vasa vasorum* for retaining the unchoked flow condition. In a nutshell, Equations 6(a-d) are the useful tools, highlighting the geometric and thermo-fluid dynamics parameters, for maintaining an unchoked flow condition in the circulatory circuit for negating the risk of AHS. It is important to note that an overdose of blood-thinning drug for reducing the blood-viscosity augments *Reynolds number* leading to high-turbulence and enhanced boundary-layer-blockage (BLB), which increases the chances of cavitation and the *Sanal-flow-choking* leading to the shock wave and pressure-overshoot causing *memory effect* (stroke history) in viscoelastic vessels. Therefore, designing the precise blood-thinning regimen is vital for attaining the desired therapeutic efficacy and negating undesirable flow-choking leading to AHS. Briefly, the analytical models reveal that the relatively high and low blood viscosity are risk factors of AHS.

It is a well ascertained physical condition in the compressible flow theory that supersonic flow will be developed in the divergent region of a choked CD duct flow passage similar to an artery with divergent or bifurcation or vasospasm regions (see Figure 1 as the central illustration). At this physical situation<sup>[1,84]</sup> there is a possibility of shock wave generation and pressure-overshoot, causation of asymptomatic aneurysm and/or AHS as the case may be.<sup>[1,37]</sup>

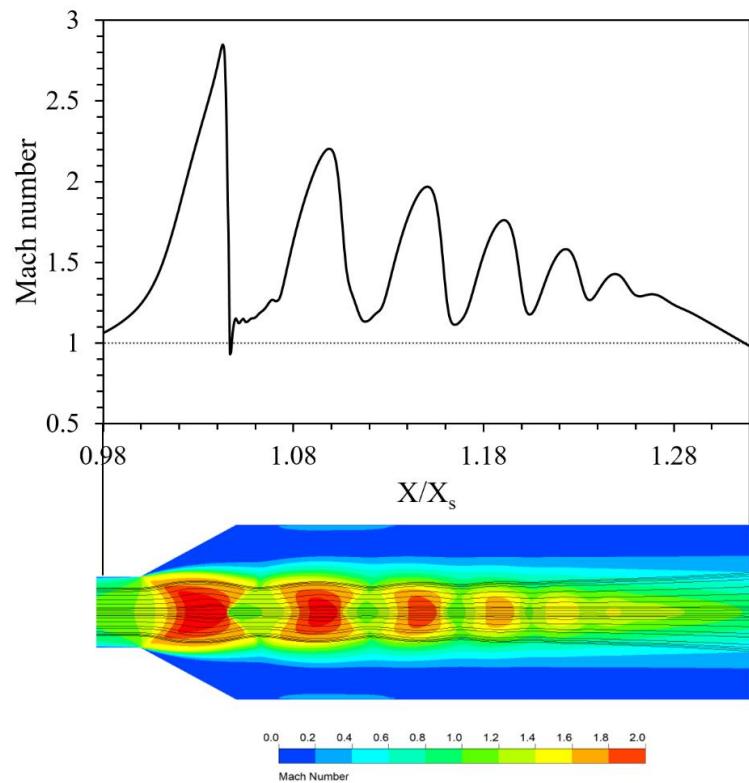
Largely, in the HCS the flow is laminar and it becomes turbulent due to blood thinners and/or due to local or seasonal effects. Note that the over dose of anticoagulant drugs decrease the dynamic viscosity of blood dramatically and as a result *Reynolds* number increases leading to enhanced BLB causing the Sanal flow choking. The flow turbulence increases the loss of energy in the form of friction, which augments the blockage factor in the vessels and generates heat and enhance the internal energy resulting a reduction in the blood/biofluid heat capacity ratio (BHCR). The flow turbulence augments the perfusion pressure vital to push the flow of blood, leading to

internal flow choking and shock wave generation. It leads to establish that at a CPR in any straight duct ending with the sudden expansion / divergent / bifurcation region could lead to detonation at a low subsonic inflow condition.

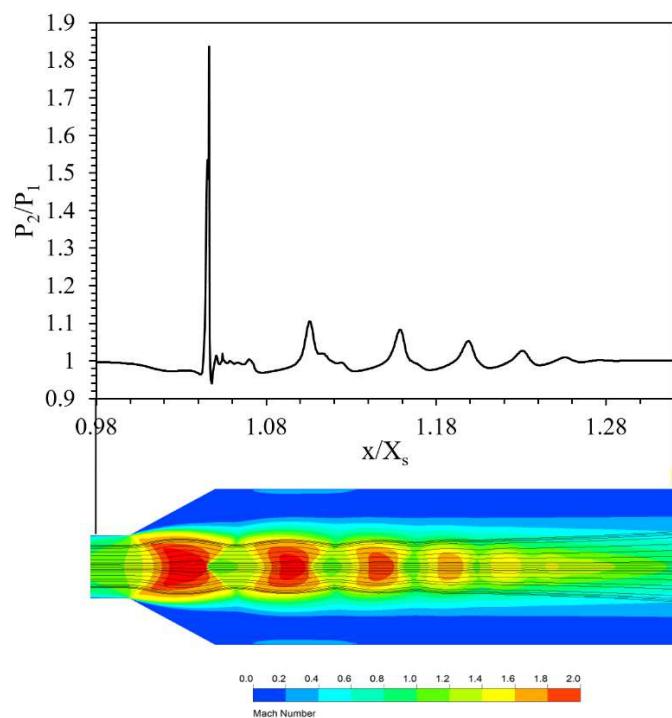
It is crystal clear from the *SANAL chart* given in Figure 5 (the solution curve of Equation 1) that, irrespective of the percentage of blockage factor, the risk of detonation could be negated by retaining the total-to-static pressure ratio in a fluid flow system always lower than LCDI. Similarly, irrespective of the percentage blockage of any artery, the risk of AHS could be reduced by maintaining the SBP/DBP ratio lower than LCHI, which is a unique function of HCR. For instance, if an internal flow system is having 50 % port area blockage, there will NOT be any possibilities of the *Sanal flow choking* leading to detonation or *hemorrhage* provided the system maintains a flow Mach number lower than 0.3 or  $BPR < LCHI$ . The upper critical hemorrhage index (UCHI) could be estimated from the HCR of blood. At a CPR, the *Sanal flow choking* would occur in a vessel with gas embolism (i.e., when  $BPR > LCHI$ ) or without gas embolism (i.e., whwn  $BPR > UCHI$ ) irrespective of the blockage factor (plaque and/or boundary layer blockage). In a nutshell, Figure 5 is explicitly showing the condition of DDT and ASH in an internal fluid flow system of any scale at the *Sanal flow choking* condition.

## In silico Results

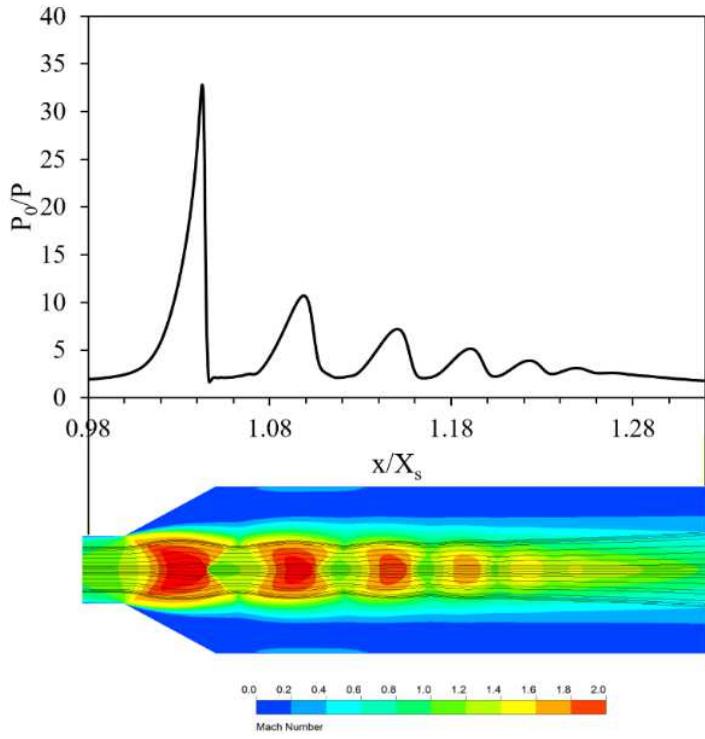
For demonstrating the proof of the concept of the Sanal flow choking and streamtube flow choking in a classical fluid flow system *in silico* studies have been conducted using a validated flow solver.<sup>[3,4,85]</sup> The results generated from the *in silico* modeling (see Figure 6(a-c) and Figure 7(a-f)) are conveying the message to the scientific community on the occurrence of the *Sanal flow choking* and streamtube flow choking in a diabatic fluid flow system leading to detonation and asymptomatic stroke. Please see **movies S3 and S4** containing the *in silico* results.



(a)



(b)

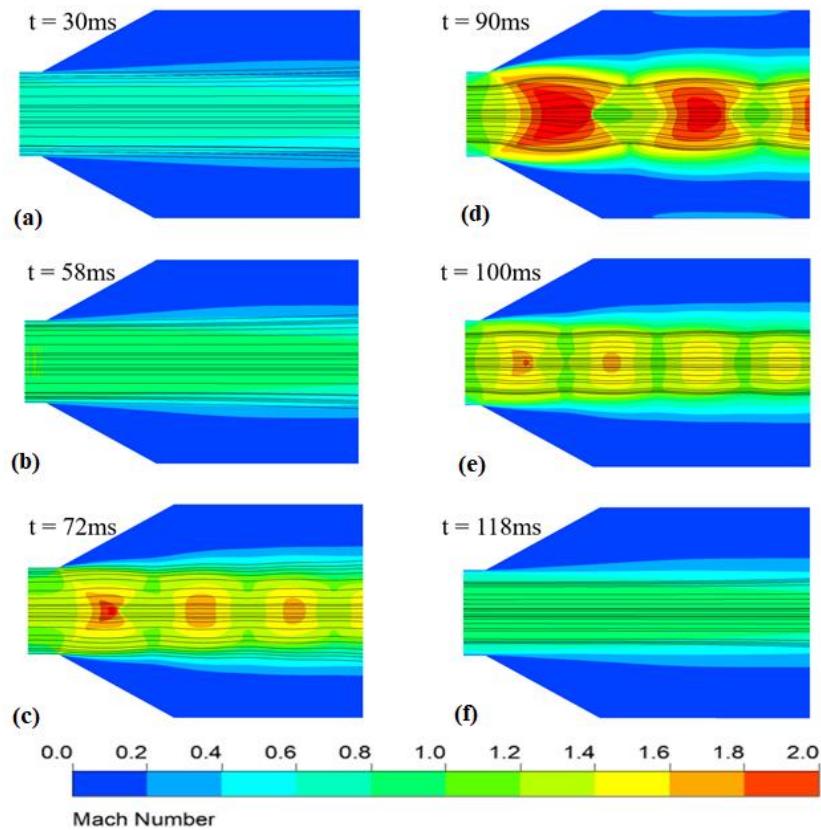


(c)

**Figure 6 (a-c)** Demonstrating the shape of the streamtube, Mach number variations, pressure ratio variation, and the detonation region during the Sanal flow choking condition (enlarged view at  $t = 90$  ms).

It is appropriate to mention here that, the simulation of chemical reaction mechanisms containing shock waves and detonation reported in the open literature are not unique.<sup>[2]</sup> Therefore, we deliberately set aside the reacting flow simulation in this fundamental pilot study for establishing one of the basic causes of DDT in the internal chemical fluid flow system. **Figure 6(a-c)** and **Figure 7(a-f)** show the *in silico* result highlighting the axial Mach number variations, sharp pressure spike and diminishing shock waves at the downstream region of the duct with bifurcation due to the *Sanal flow choking* and *streamtube flow choking*. Note that in the HCS, the large BPR oscillations could lead to the choking and unchoking phenomena creating high risk to the subjects (human being / animal) leading to an *arrhythmia*. Due to the periodic *Sanal flow*

*choking* any valve, including heart valve, with CD duct shaped flow passage will get more defects than convergent type valves as time advances in any flow circuit. This is corroborated with the clinical findings.<sup>[1,7,8]</sup> The fact is that during the *Sanal flow choking* the divergent region of the valve will experience the shock wave and pressure overshoot causing damage. Most heart valve problems involve the aortic and mitral valves, possibly because of its geometric shape similar to CD duct flow passage. The valve defects can happen in water pipe line due to cavitation and shock waves.<sup>[1]</sup> Further discussion on the defects of various types of valves is beyond the scope of this article.



**Figure 7(a-f)** Demonstrating the shape of the streamtube and the Mach number contours at different time intervals before and after the Sanal flow choking (enlarge view of the transition region).

Figures 7(a-f) are showing the enlarged view of the streamtube, demonstrating the shape of the streamtube and the Mach number contours at different time intervals before and after the Sanal flow choking. It is crystal clear from Figure 6 and Figure 7 that the streamlines are compressed and the pressure differences are significant within the streamtube and as a result the flow gets enhanced to the narrow region of the streamtube for satisfying the conservation law, which leads to *Sanal flow choking* and detonation due to the convergent-divergent (CD) shape of the streamtube. Normal shock and oblique shock waves are evidenced in the *in silico* results. The Sanal flow choking location, the strength of shock, and shock diamonds can be observed in Figure 6(a-c). Packed streamlines could be discerned in the constricted area of the streamtube (see Figure 6(a-b) and Figure 7(a-f)) where low pressure is evident. In the case of biological flows, the *sonic-fluid throat* location discerned in Figure 6(a-c) could alter due to the BPR oscillation, wall flexibility of the viscoelastic blood vessel, chemistry of multi-species and multiphase fluid flow, and pathophysiological conditions.

The objective of this study was to establish the phenomenon of the Sanal flow choking and streamtube flow choking through the *analytical* and *in silico* modeling of diabatic fluid flows, which we could achieve herein. In the case of HCS, the blood and/or biofluid could get evaporated at the higher temperature creating an undesirable formation of gases within the duct creating a detrimental *flow choking* due to low HCR of the evolved gas leading to gas embolism.<sup>[1-9]</sup> Figure 6(a-c) and Figure 7(a-f) are analogous to biofluid choking effect in the circulatory circuit due to gas embolism. Briefly analytical and in silico results established that predicting the conditions of LCDI and LCHI, based on the lowest HCR of evolved gas, are inevitable for negating the undesirable DDT and ASH in any fluid flow system with credibility.

## Concluding Remarks

The theoretical discovery of Sanal flow choking received considerable attention in the audience of Physics of fluids, chemical and central science for resolving centuries long unresolved problems. Understanding flow physics and chemistry, and the transport of fluid from creeping inflow to the supersonic flow at the *yocto* to *yotta* scale systems are of significant interest for testing classical theories of the continuum and non-continuum fluid flows for solving varieties of industrial problems with credibility. Gotthard Seifert<sup>[102]</sup> reported *ab initio* *in silico* simulations, which provide a sign of the development of the molecular and electronic structure of an explosive undergoing detonation. Moseler and Landman<sup>[103]</sup> used molecular dynamics (MD) simulations of nanoscale jets to encounter a rupture profile not illustrated by macroscopic theory. Of late (2020), Chengxi Zhao<sup>[104]</sup> reported that the soundness of the traditional theories at the microscale and nanoscale has been taken into question. Authors reported that the thermal fluctuations are spontaneously occurring within molecular dynamics (MD) simulations. D.M.Holland et al.<sup>[105]</sup> further reported that the time dependent mass flow rate predicted using their enhanced *in silico* simulation matches well with full molecular dynamics (MD) simulation and highlighted that the traditional *in silico* results of such cases are incompetent. It leads to say that in real world scientific experiments of complex nano-microscale systems the robustness of *in silico* model needs to be tested to featuring the actual fluid characteristics in a non-trivial geometry at the *nanoscale*. Singh and Myong<sup>[106]</sup> reported that for improved modeling efforts, the joint effect of material properties, the scale and shape of the flowing medium on fluid flow must be taken into account, which we conclusively addressed herein through the closed-form analytical models capable to solve real-world fluid flow (continuum / non-continuum) problems experiencing *deflagration to detonation transition* of any scale.

The physics of detonation chemistry presented herein through the Sanal flow choking/streamtube flow choking phenomenon is a pointer for predicting detonation in *yocto* to *yotta* scale systems and beyond, which includes environmental and supernova explosions.<sup>[107, 108]</sup> Note that the mechanism whereby a degenerate carbon-oxygen white dwarf explodes, producing a *Type Ia supernova* (SN Ia), still remains poorly understood.<sup>[109]</sup> Earlier researchers do not know whether the burning wave propagates through the white dwarf as a supersonic detonation or as a subsonic deflagration.<sup>[108-122]</sup> Herein, we provide the proof of the concept of the Sanal flow choking and streamtube flow choking causing the sharp pressure spike due to shock wave formation. The streamtube flow choking is a radical theory in predicting the deflagration to detonation transition in both internal and free external flows. At the low subsonic inlet conditions, the real-world fluid flow (continuum / non-continuum) system with the divergent/bifurcation duct could incline to *deflagration-to-detonation-transition* (DDT) due to the phenomenon of the boundary-layer-blockage (BLB) factor induced the *Sanal flow choking* in a wall-bounded or streamline bounded flows at a critical pressure ratio. The *Sanal flow choking* is vulnerable to catastrophic failures of reacting and non-reacting fluid flow systems with sudden expansion/divergent port due to the cavitation, shock wave and detonation as the case may be. At the lower critical detonation or hemorrhage index, the critical pressure ratio of the chemical energy system and the blood pressure ratio (BPR) of the subjects (human being / animal) are unique functions of the heat capacity ratio (HCR) of the gas in the duct. *Numerical simulations are* carried out with creeping inflow conditions using a calibrated viscous flow solver<sup>[3]</sup> for demonstrating the novel concept of the *fluid-throat* induced *Sanal flow choking* followed by the shock wave generation and pressure overshoot in a straight-tube ending with a divergent port, similar to an artery with the divergent / bifurcation region. We concluded that the detonation kernel is more sensitive in the reacting flows

generating the leading species with low HCR. We also concluded from the analytical solution that the biofluid / blood with low HCR is more susceptible to *asymptomatic hemorrhagic stroke* (AHS) in the circulatory circuit of all subjects due to an early *flow choking*. The risk of *Sanal flow choking* and streamtube flow choking could be negated by breaking the blockage and/or increasing the HCR of the evolved gases in the tube for keeping the total-to-static pressure ratio always lower than the lower critical detonation / hemorrhage index in any fluid flow system. *In silico* results reported herein shed light for the biological, chemical, energy, environmental, material and aerospace systems design and drug discovery. The result of this study is a strong exposition to the industry for the elimination of the detonation in any energy system with confidence, which was an unknown fact to the scientific communities for several decades.<sup>[1-4, 86-91]</sup>

Using the exact solution reported herein a detonation free energy system could be devised authoritatively by regulating the inflow condition, selecting the fluid viscosity, HCR and the average wall-friction coefficient based on the upstream length-to-diameter ratio of the flow system for achieving the condition  $LCDI > (P_{total}/P_{static})_{fluid-throat}$ . In other words, we can reduce the risk of DDT by increasing the HCR. In the case of biological systems by keeping  $BPR < LCHI$ , we could reduce the risk of AHS.<sup>[1-9]</sup> It can be achieved by increasing the BHCR, which could simultaneously reduce blood viscosity and turbulence. A fluid-structural simulation could be useful to offer cogent answers to clinical questions pertaining to AHS and *aneurysm*, which are beyond the scope of this manuscript. In a nutshell, this basic research article sheds light for discovering the likelihoods of *biofluid flow choking*, *Sanal flow choking* and *Streamtube flow choking* in real-world fluid flow system [123-125]. Briefly, analytical, and *in silico* results highlighted in this article will complement preclinical *in vivo* assessments in *mega* and *nanotubes* and can fine-tune decision making steps in biomaterial design and drug discovery through the

*nanotechnology*.<sup>[89-101]</sup> This article is a part of the scientific odyssey that resulted from a collaboration among members from various research groups, viz., rocket propulsion, physical and material science, chemical science, environmental science, biomaterials, biomedical, cardiology, nanotechnology and nanomedicine.

## **Supplementary Materials**

**Movie S1:** In vitro result demonstrating the shock wave generation in a viscoelastic tube with vasospasm at a critical pressure ratio: <https://youtu.be/59E6pI3L5Rc>

**Movie S2:** In vitro result demonstrating the internal flow choking and the shock wave generation in a viscoelastic tube with vasospasm at different locations at a different pressure ratio: <https://youtu.be/UQqtpQaUVHg>

**Movie S3:** In silico result demonstrating the boundary layer blockage induced the Sanal flow choking at a critical pressure ratio: [https://youtu.be/eFndUAU\\_m5I](https://youtu.be/eFndUAU_m5I)

**Movie S4:** *In silico* result demonstrating the phenomenon of the *stremtube flow choking* in an internal flow system at a critical pressure ratio: <https://youtu.be/bv3ZDcPKMSI>

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## **Data availability**

The raw data required to reproduce the *in silico* results are available with the corresponding author and could be shared on request.

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# Figures

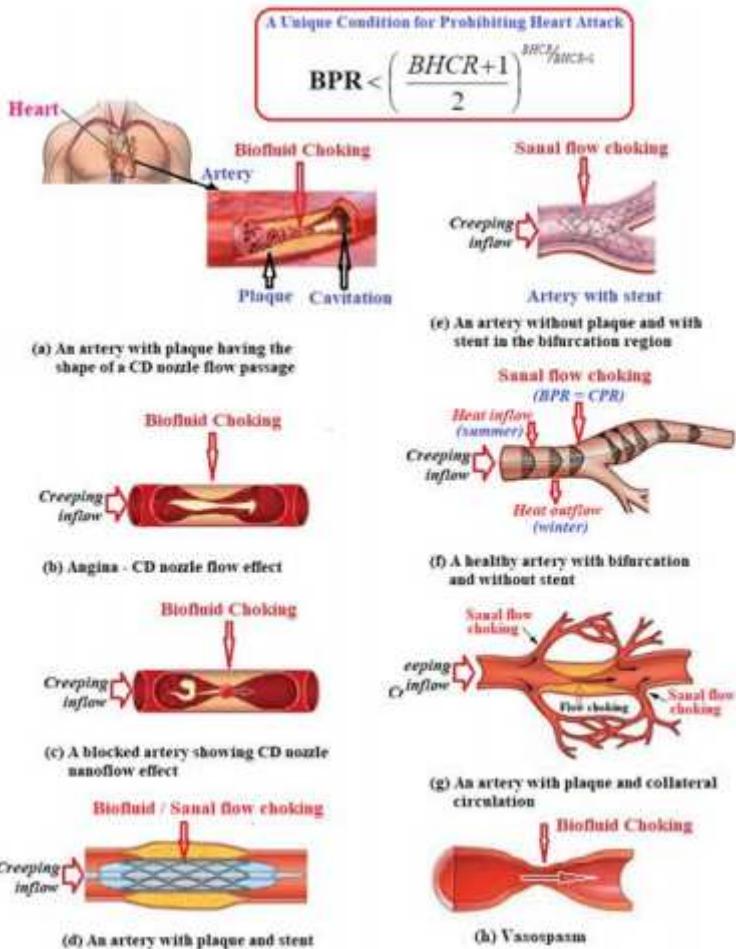
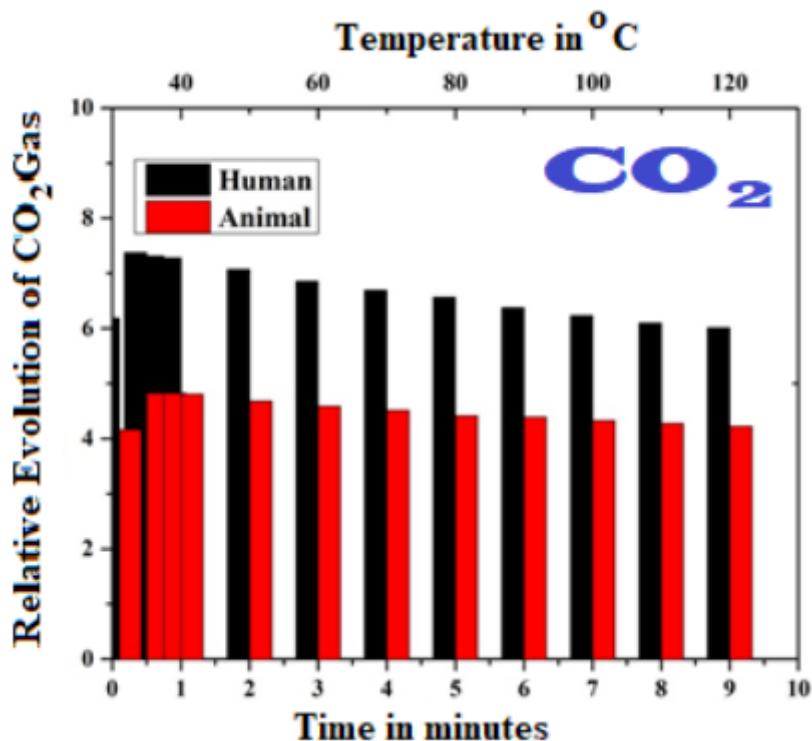


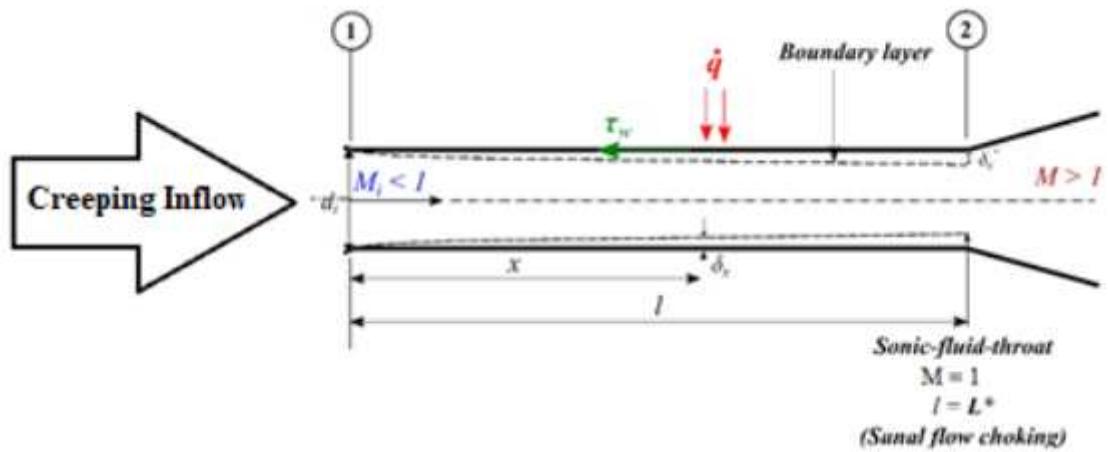
Figure 1

(a-h). Internal flow choking in HCS (The Central Illustration) [1]



**Figure 2**

In vitro result shows the mass spectrum of carbon dioxide (CO<sub>2</sub>) evolved as a function of both time and temperature in blood samples of healthy subjects at 37-400 C (98.6-1040 F) and beyond the physiological range (the human being / Guinea-pig) [5].



**Figure 3**

Demonstrating the Sanal flow choking condition in an internal fluid flow system.

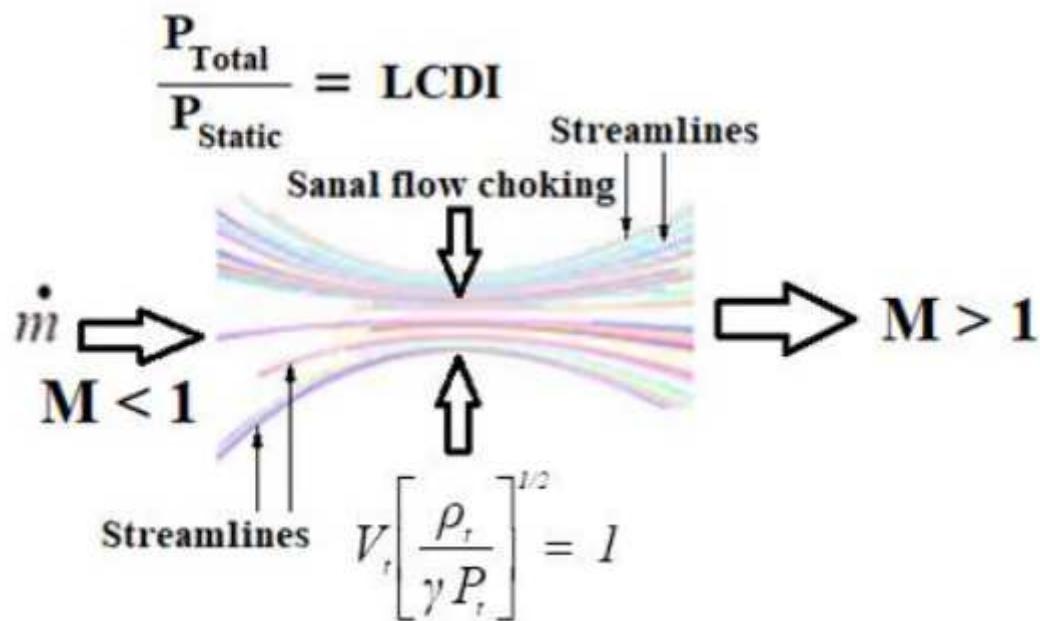
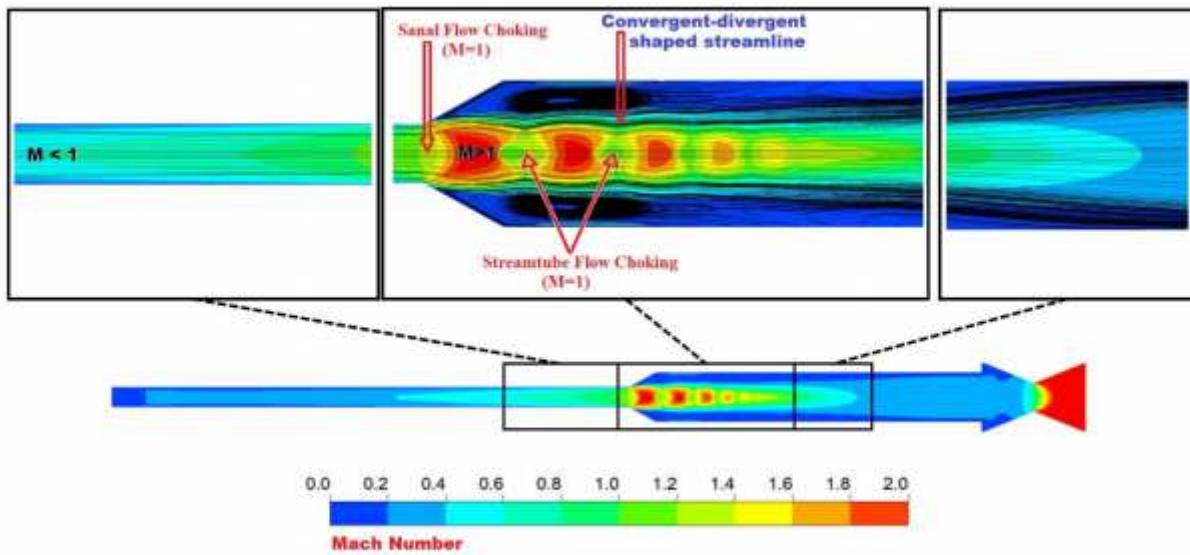
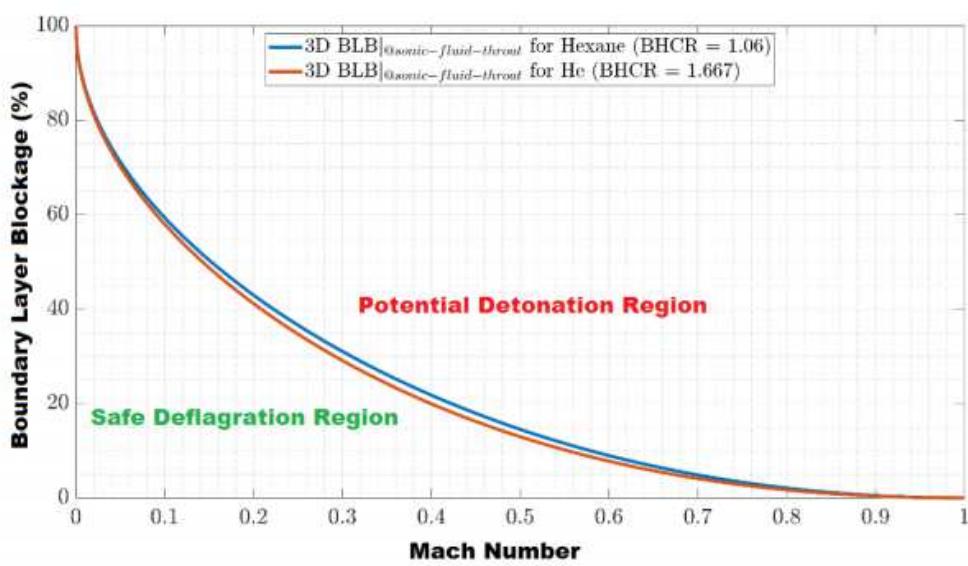
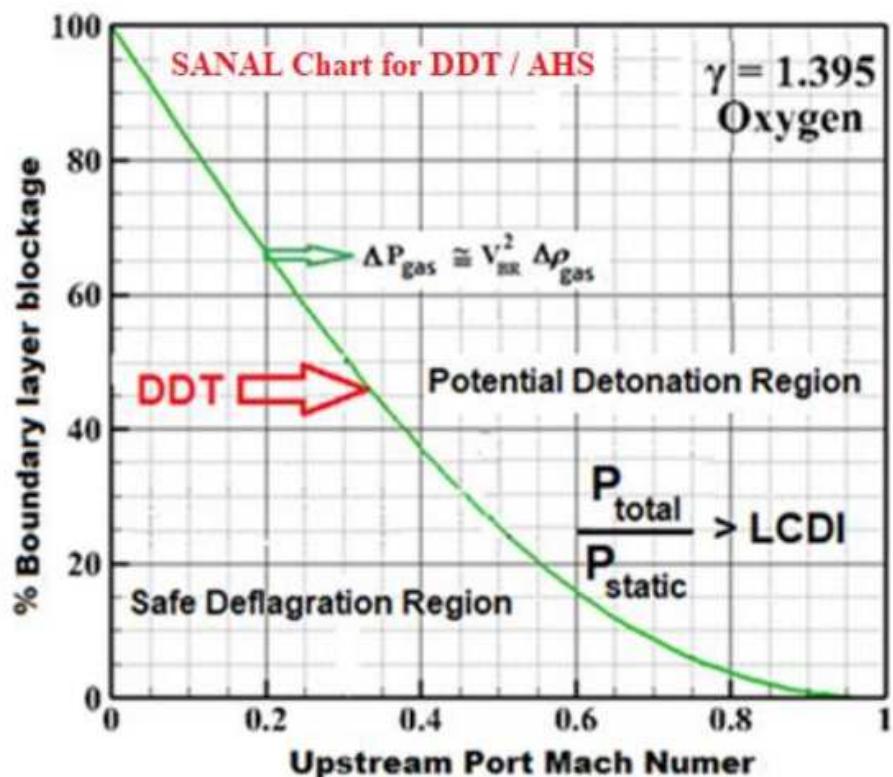


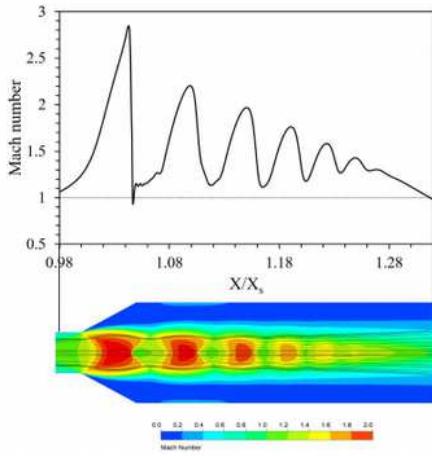
Figure 4

(a). The enlarged view of the Sanal flow choking and the streamtube flow choking phenomena in an idealized physical model of an internal fluid flow system <Movie: <https://youtu.be/bv3ZDcPKMSI>>. (b). Demonstrating the CD duct flow effect in yocto to yotta scale internal and external flow systems leading to streamtube flow choking.

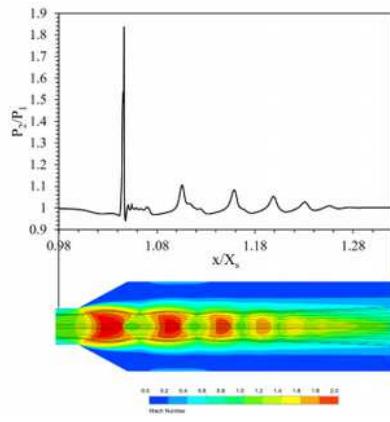


**Figure 5**

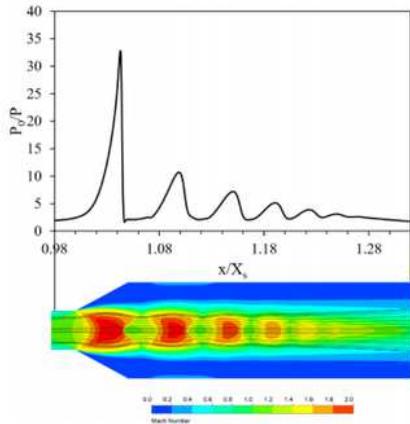
- (a). Demonstrating the condition of DDT and AHS in an internal flow system at the Sanal flow choking condition (2D case). (b). Demonstrating the condition of DDT in an internal flow system at the Sanal flow choking condition for two different gases (3D case).



(a)



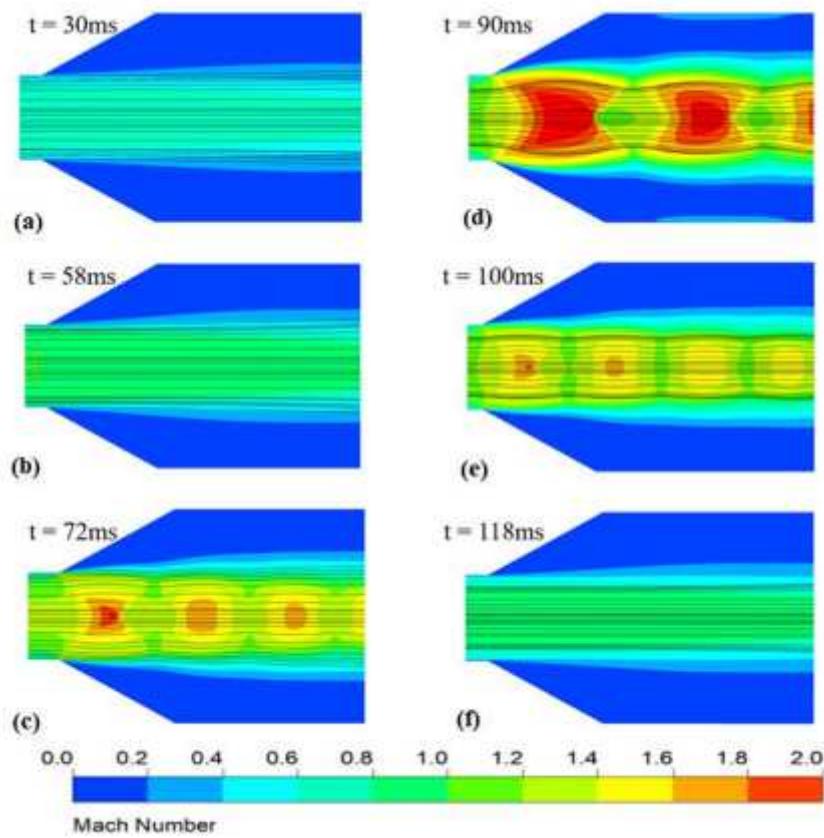
(b)



(c)

**Figure 6**

(a-c) Demonstrating the shape of the streamtube, Mach number variations, pressure ratio variation, and the detonation region during the Sanal flow choking condition (enlarged view at  $t = 90$  ms).



**Figure 7**

(a-f) Demonstrating the shape of the streamtube and the Mach number contours at different time intervals before and after the Sanal flow choking (enlarge view of the transition region).