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Divergence Half-Angle Optimisation in Conical De Laval Nozzles: Reconciling CFD and Experimental Disagreements Through Nozzle Pressure Ratio Analysis

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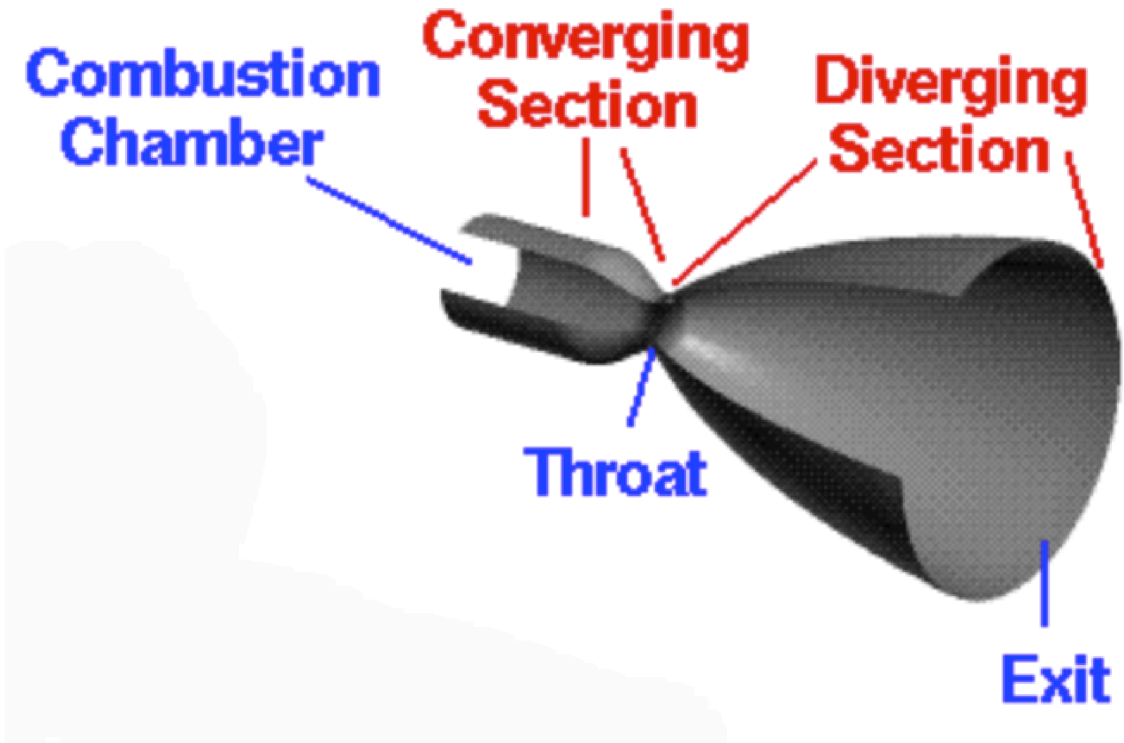
ABSTRACT

The divergence half-angle of a convergent-divergent nozzle is the primary geometric determinant of thrust performance, yet current literature reports optimal angles ranging widely with no consensus and no agreed explanation for this spread. This review investigates whether the disagreement can be explored through a single governing variable: Nozzle Pressure Ratio (NPR), the ratio of chamber to ambient pressure that varies continuously as a rocket ascends. Combining analytical derivations from the thrust equation, numerical solution across a range of operating conditions, and a synthesis of fourteen hybrid studies organized by NPR regime, the paper establishes that the thrust-optimal divergence angle is not a fixed geometric constant but increases with NPR. The reviewed studies confirm this predicted trend while sitting systematically above the idealized theoretical curve, and experimental optima consistently exceeds computational predictions at matched NPR, indicating systematic conservatism in prevailing CFD methods. The review provides directionality, but further quantification is necessary, specifically in the transitional NPR regime.

INTRODUCTION

In today's field of aerospace and rocketry, propulsion efficiency has become a pivotal factor in rocket design, wherein thrust performance translates to payload capacity, range, fuel burn and costs. As the industry confronts the environmental costs of aviation and spaceflight, and as sustainable jet fuel remains expensive and supply-intensive, extracting more thrust from existing propellant through optimized engine and nozzle design provides an alternative path to reducing fuel burn and emissions. This field of research is extremely fundamental to the aerospace sector as design optimization is the key driver of the space economy, enabling routine commercial access to space, and advanced satellite deployment (Serrano). And at the centre of this efficiency lies a single, decisive component: the nozzle.



(NASA, "Nozzle Design - Converging/Diverging (CD) Nozzle")

A nozzle is a small, but crucial component of the engine system, that acts to conduct exhaust gases into the free stream (airflow outside the system), to produce thrust that contributes to the rocket/jet system's acceleration in the opposite direction of the removal of these gases. Nozzles come in various geometries. However, throughout this review, we will be considering the Convergent-Divergent (CD) Nozzle, which is often called the de Laval Nozzle. In this nozzle, the flow first converges down to the minimum area or throat, then is expanded through the divergent section to the exit at the right (Hall). These nozzles are heavily used in the aerospace industry due to their efficient engine operation (Hall, "Nozzles").

Specifically speaking, the divergence half -angle of a CD nozzle acts as the primary geometric lever on thrust performance. Even a slighter change in the slant of the diagonal in the divergence sector, and thrust performance is immensely influenced. Thus finding an optimal divergence angle for each set of nozzles in different environmental and operating regimes is pivotal to increase efficiencies of our systems. However, existing literature reports varying divergence angles – between 11° to 30° – with no verified consensus and no agreed explanation for the spread. This raises questions such as methodological completeness, experimental validation and performance metrics. Regardless of how multifactorial rocket design is, the most overlooked, yet crucial variable is the Nozzle Pressure Ratio (NPR) regime.

This review, aims to address the spread of the optimal divergence half angle, with respect to the NPR regime, to establish a meaningful relationship between the two, and hence increase the understanding of the influence of environmental conditions on the optimal angle. Through this lens, the paper aims to provide a unique perspective on rocket design, that no existing literature traces, as well as clear disagreements between physical experimentation and computational analysis, that is CFD models. The review's approach towards discussing these strands would be pragmatic: starting from theoretical derivations to discussion of the case studies to numerical analysis and finally towards the deviations in practical literature away from theoretical concepts.

ANALYTICAL DERIVATION

The following derivation proceeds under the assumption of isentropic, ideally perfect gas flow , which neglects viscous losses, heat transfer, and real-gas effects. This idealisation is what causes the resulting theoretical curve to deviate from the data in Figure B, a point developed in Section 4.

The general equation that governs thrust generation in the CD Nozzle is the following:

$F = \frac{m}{t} \bullet v_e + A_e(P_e - P_o)$ (Hall, "Thrust Equation")

However, in the CD Nozzles, the exhaust gases are directed towards an angle called the divergence angle, because of which not all particles travel perfectly parallel to the centerline of the nozzle. To be precise, the flow of particles becomes non-axial in a CD Nozzle, because of which not all kinetic energy contributes to forward thrust, which is an axial quantity. Due to these losses, a correction factor is applied to the thrust equation that gives a more accurate computation of the effective thrust produced. λ, is used to denote the loss in the efficiency of the nozzle and is defined by the equation:

$$\lambda = \frac{1+cos(\alpha)}{2} \; wherein \; \alpha \; is \; the \; divergence \; half - angle$$

(Sun et al.)

This gives us the updated equation for the thrust generated:

$$F = \frac{m}{t} \bullet v_e\lambda + A_e(P_e - P_o)$$

To investigate the effect of the divergence angle on the efficiency of the thrust generated, a dimensionless quantity Thrust coefficient, C_T is introduced.

$$C_T = \frac{\lambda \bullet m \bullet v_e}{t \times P_C A_T} + \left(\frac{P_e}{P_C} - \frac{1}{NPR}\right)\left(1 + \frac{L}{r_T} tan(\alpha)\right)^2 \text{ (Berton)}$$

Wherein, P_C represents Chamber Pressure, A_T represents throat area, L represents the horizontal; length of the diverging section, and r_T represents the radius of the Throat.

When NPR falls below its design value, the exit pressure drops below the ambient pressure. To equalize with the ambient pressure, oblique shock waves are created in the diverging section, creating highly asymmetrical turbulent airflow. This is called the overexpanded condition, and it converts supersonic kinetic energy into pressure and heat at the cost of thrust efficiency. When NPR is greater than the design value, the exhaust gases expand radially, in what's called the under-expanded condition (Utah State University)

The thrust coefficient as presented, if fully determined by two variables, the divergence half angle – which governs the mass flow rate, exit velocity, the loss factor and the Pressure terms – and the Nozzle Pressure Ratio, NPR. All other terms are geometric consequences of α rather than independent parameters. This structure reveals that for the maximum thrust generated, the α doesn't work in isolation as any shift in the NPR alters the pressure components that are independent of the nozzle geometry, producing varying optimum angles at which thrust is maximized.

To find the optimal angle in the CD nozzle, differentiation would have to be applied to the thrust coefficient equation and then that should be set to zero, to find the optimal angle. Below is the clean analytical derivation alongside an explanation and computational analysis.

The thrust-optimal divergence angle is found by differentiating the thrust equation with respect to α and then setting it equal to zero:

$$\frac{dC_T}{d\alpha} = \frac{d}{d\alpha}\left[\frac{\lambda \bullet m \bullet v_e}{P_C A_T} + \left(\frac{P_e}{P_C} - \frac{1}{NPR}\right)\left(1 + \frac{L}{r_T} tan(\alpha)\right)^2\right] = 0$$

Which yields the full optimization conditions:

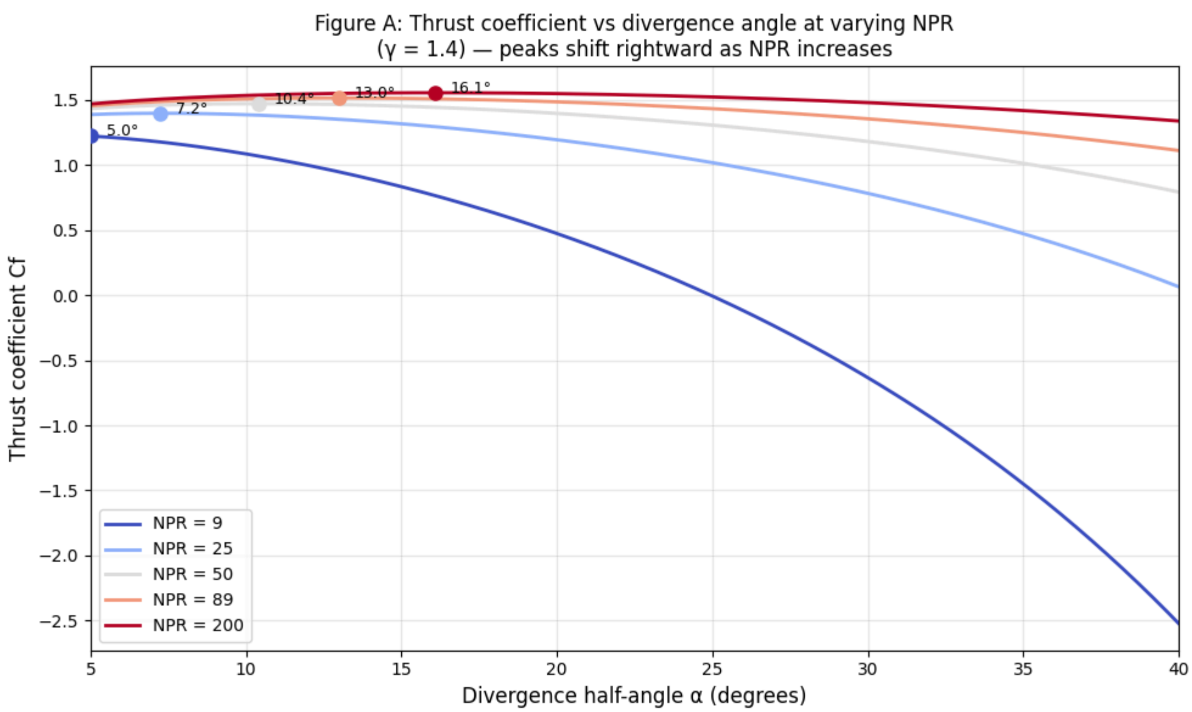
$$-\frac{mv_e}{tP_c A_t} \cdot \frac{sin(\alpha)}{2} + \left(\frac{P_e}{P_C} - \frac{1}{NPR}\right) \cdot 2\left(1 + \frac{L}{r_T} tan(\alpha)\right)\frac{L}{r_T} sec^2(\alpha) = 0$$

Looking at the geometric derivative factor, one containing tan(α) and sec(α), will always be greater than zero as $0° < \alpha < 90°$, and hence the governing term for the right hand product would be $\left(\frac{P_e}{P_C} - \frac{1}{NPR}\right)$. Thus, NPR controls the optimum angle found.

At low NPR, the $\frac{1}{NPR}$ is too large, meaning that $(\frac{P_e}{P_c} - \frac{1}{NPR})$ is negative. And hence term 2 would always be negative paired with the permanent negative derivative of term 1. The implication of this is that the value of C_T has been negative from the start, because of which the optimum is found at smaller α, meaning that α is not allowed to grow. Whereas, At high NPR, 1/NPR approaches zero, so the bracket becomes positive. Term 2's derivative is now positive and grows with α . This positive pressure contribution competes against Term 1's negative momentum contribution. The optimum is the angle where they exactly balance and because the positive term strengthens as NPR rises, that balance point shifts to larger α.

However, the balancing condition has no closed-form solution because the pressure and momentum terms cannot be algebraically separated. It is therefore, computed across a range of values of NPR in Fig A, which plots the thrust coefficient, C_T, against divergence angle, α, and identifies the optimal angle at each condition as the peak of each curve.

Figure A



The rightward shift of the curve's peaks represent the clean analytical hypothesis made above: the thrust-optimal divergence angle is directly proportional to the NPR operating regime.

CASE STUDIES

The theoretical framework established earlier, predicts that the optimal divergence angle, with respect to the maximum thrust coefficient, consistently increases with the NPR as the pressure terms begin to dominate at higher operating chamber pressures. The following section will examine existing CFD and experimental literature to predict whether they reflect the prior-made derivations, organizing the evidence by NPR regime, method used and the key tensions that arise from these cases.

Figure B presents the thrust optimal divergence angle versus the NPR relationship derived in section 2, overlaid with 14 data points from CFD and experimental literature.
Figure B:

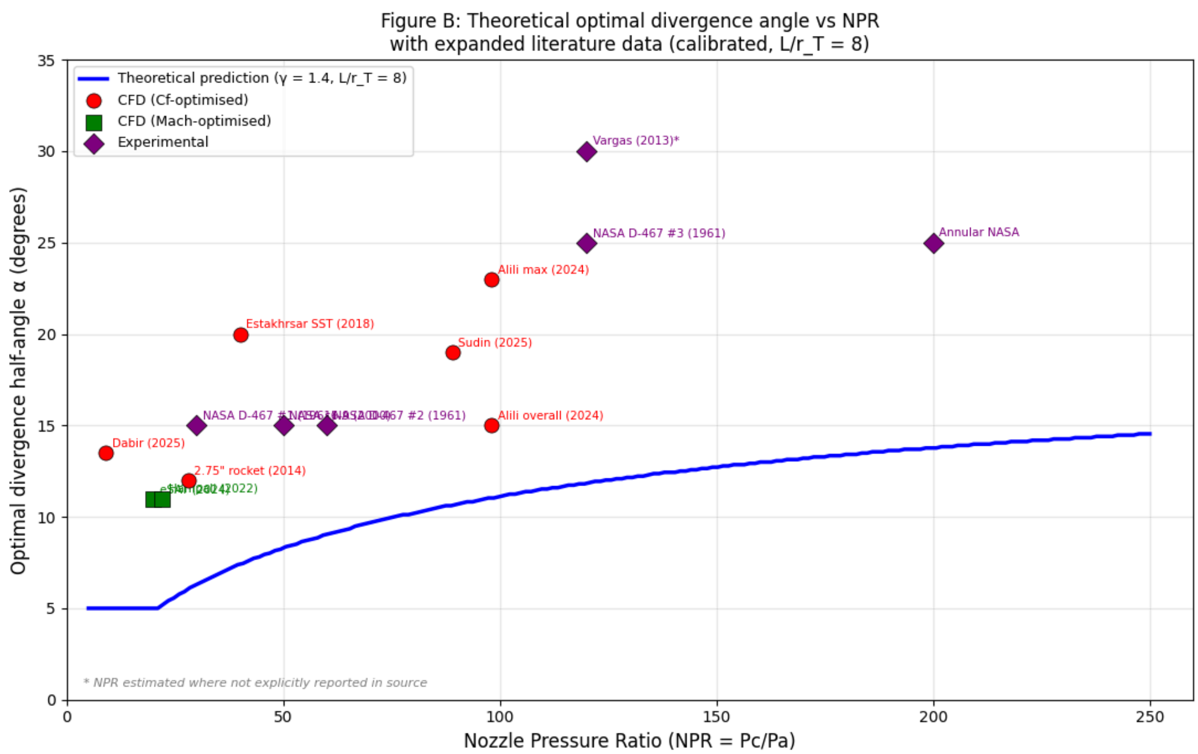


Figure B represents the Theoretical optimal divergence half-angle vs NPR (solid curve, γ = 1.4, calibrated L/r_T = 8), which is overlaid with fourteen CFD and experimental data points. Methodology categories: CFD thrust-optimised (red circles), CFD Mach-optimised (green squares), experimental (purple diamonds). The trend formed in Fig B, confirms to the systematical directional argument made in section 2: as NPR increases, the optimal angle favoured starts to increase. This also confirms the analysis made from Fig A.

Data points marked with an asterisk (*) denote studies that did not explicitly report NPR. Their positions on the NPR axis were estimated from their reported operating conditions. Where chamber and ambient pressures were given, NPR was computed directly as their ratio. On the contrary, where only inlet pressure and operating altitude were reported, ambient pressure was inferred from the International Standard Atmosphere model and NPR was derived accordingly. For Vargas (2013), a high-NPR condition was estimated from the lab-scale hybrid rocket chamber pressure and near-atmospheric exhaust; for Hampali (2022), NPR was inferred from the reported area ratio and design expansion condition.

The ratio L/r_T , which relates the divergent-section length to the throat radius, and essentially sets the height of the theoretical optimal-angle curve. For any nozzle reporting both an area ratio ε and divergence angle α, it follows that $\frac{L}{r_T} = \frac{\sqrt{\varepsilon}-1}{tan(\alpha)}$; applying this to the conical studies in the evidence set yields values between roughly 6.3 and 9.6, with a median set near 8. Across this physically justified range the predicted optimal angle shifts by only a few degrees, and its continuous increase with NPR, which is the study's central argument, is preserved throughout. The calibration therefore governs the curve's absolute height but not its qualitative behaviour, and the empirical points in Figure B remain systematically above it even at the upper end of the range, confirming the offset is genuine rather than artificial.

Table 1 : Literature Data Points (Figure B Overlay)

Study	Year	Method	Metric	NPR	Optimal α (°)	Area ratio ε
Dabir	2025	CFD	C_T	9	13.5	—
Swaroopini	2024	CFD	Mach	20	11.0	~3.9
Hampali	2022	CFD	Mach	22*	11.0	—
2.75″ rocket study	2014	CFD	C_T	28	12.0	—
Estakhrsar (SST)	2018	CFD	C_T	40	20.0	~10
Sudin	2025	CFD	C_T	89	19.0	—
Alili (overall)	2024	CFD	C_T	98	15.0	—
Alili (max thrust)	2024	CFD	C_T	98	23.0	—
NASA TN D-467 #1	1961	Exp	Thrust ratio	30	15.0	10

NASA TN D-467 #2	1961	Exp	Thrust ratio	60	15.0	25
NASA TN D-467 #3	1961	Exp	Thrust ratio	120	25.0	40
NASA ε6-9	2000	Exp	Thrust ratio	50	15.0	6–9
Annular nozzle (NASA)	—	Exp	Thrust ratio	200	25.0	25
Vargas	2013	Exp	Thrust force	120*	30.0	—

While Figure B incorporates fourteen studies to establish the aggregate optimal-angle-versus-NPR trend across the breadth of the available literature, the detailed analysis that follows focuses on six core studies selected for their methodological completeness, with each reporting the divergence-angle range tested, operating NPR, performance metric, and turbulence model in sufficient detail to permit individual examination . These six, spanning the low- and high-NPR regimes, are summarised in Table 2.

Table 2:

Author & Year	Method	Angle Range Tested	NPR	Claimed Optimal Angle	Performance Metric	Regime
Dabir	CFD	5-13.6	9	13.5	Thrust Coefficient	Low NPR
Swaroopini	CFD	7-50	17.46-24.72	11	Mach Number	Low NPR
Hampali	CFD	5-20	Not stated	11	Thrust Coefficient	Low NPR (inferred)
— No studies identified in this NPR Range —						
Sudin	CFD	7, 13, 19	High	19	Thrust Force (lbs)	High NPR
Alili	CFD	10-25	89-1000	15	Thrust	High NPR

					Coefficient & Specific Impulse (Isp)	
Vargas	Experimental: Hybrid Rocket; lab scale	15,30	Lab scale testing	30	Thrust Force (lbs)	High NPR

Notably, when the six core studies are arranged by operating NPR, they cluster at the low-NPR (9–25) and high-NPR (89 <) extremes, with none falling within the intermediate NPR 25–89 regime. While the broader literature surveyed in Figure B does include isolated measurements at these intermediate pressure ratios, none reports a high quality methodological detail: the full divergence-angle sweep at a defined NPR, which is required to resolve how the optimal angle behaves through this transitional band. The regime is therefore not absent from the literature but unresolved within it: no study traces the optimal-angle trajectory continuously across the pressure ratios through which a nozzle passes during ascent. This is the gap the present analysis identifies as most consequential.

Table 2 presents the case studies analysed in this review, organised by the operating regime to clarify the effect of Nozzle Pressure Ratio on the optimum divergence angle of a CD nozzle. The table separates into two subparts — Low NPR and High NPR — with no studies falling between these two ends of the spectrum, highlighting a critical research gap discussed below. Low NPR corresponds to sea-level and ground-test conditions (NPR 9–25), while high NPR corresponds to upper-atmosphere and near-vacuum operation (NPR 89–1000). The NPR 25–89 gap represents the transitional altitude band through which every rocket ascends and is also the regime where the optimum angle shifts most rapidly and where no study in this evidence set provides systematic data. This absence of cases in the intermediate regime marks the critical research gap the paper aims to address.

NPR is defined as the ratio of the total pressure inside the nozzle to the static ambient pressure and is a measure of flow expansion in nozzles. At low NPR conditions, the larger ambient pressure term drives the system to an over-expanded flow-state, because of which optimum angles are found at or below 15° (Dabir et al, Hampali et al, Swaroopini et al.). This is observed because at larger divergence angles, there is a larger pressure gradient, which induces a greater flow asymmetries and shock structures (like Mach disks or lambda shocks) as well as cause side-loads that damage the engine, that reduce the efficiency of the thrust generation (P. Nair et al.) At Low NPRs of about 9, the ambient pressure becomes so dominant that it eliminates the NPR value towards negative or zero, leaving the momentum thrust component, which is governed by the divergence loss factor, as the dominant determinant of C_T .

However, the sharpest illustration seen at this operating regime is in the case of Dabir's study. In which a CFD analysis at NPR 9 was conducted, and an optimum angle of 13.5 ° was claimed, a result which needed a careful examination. Given that Dabir's examination is terminated at 13.6° which is close to the minimum angle at which flow separation occurs (15°), it suggests that the reported optimum is not actually a mathematically proven maximum but rather ceiling constrained due to the consequences of flow separation. The separation-onset angle established by NASA's experimental data suggests that under the severe over-expansion characteristic of NPR 9, flow separation occurs at divergence angles near 15°, as the adverse pressure gradient overcomes the boundary layer at larger angles (Morrisette and Goldberg). This finding is consistent with both Hampali and Swaroopini, both of which identify angles in the range of 11–12° in the similar range of NPR values. These three studies were conducted independently, by separate research groups using distinct nozzle geometries and unrelated datasets, so their agreement does not stem from shared inputs. A limitation of these findings is that all three rely on the same k-epsilon CFD model, representing a uniformity in method that — despite their independence — limits the extent to which their agreement constitutes accuracy relative to independent experimental validation (Wilcox).

There exists a literature gap when we are considering the operating regime of an intermediate NPR, between 25-89, as no case study systematically investigates nozzle performance in this operating regime. This physical literature gap of this operating regime represents the initial phase of the rocket's ascent, wherein the ambient pressure drops to around 1000 Pa as the rocket accelerates towards the upper troposphere (Canchero). In this altitude band, the $\frac{1}{NPR}$ value continues to decrease, driving a sign change in the pressure thrust term, $\left(\frac{P_e}{P_C} - \frac{1}{NPR}\right)\left(1 + \frac{L}{r_T}tan(\alpha)\right)^2$ – from negative in the over-expanded flow regime to a positive in the ideally approaching NPR regime, wherein the larger angle increases the overall pressure thrust term – meaning that in the intermediate unstudied NPR, the thrust dependent optimal divergence angle goes through the most rapid upward shift (P. Sutton). Because of this rapidly changing divergence angle, it makes it difficult to replicate this reality through simulations or ground testing, leaving the range unprioritized by both CFD & Experimental studies. Due to this discontinuity in the evidence set, it makes it necessary to interpolate data to understand the full profile range for the rocket, which has obvious limitations as a precise value is not obtained for this intermediate operating regime, which frames this as a central unresolved problem in the optimization of the divergence angle.

At high NPR conditions, the near zero ambient pressure leads to the elimination of the $\frac{1}{NPR}$ term, as it oscillates near zero, and hence the pressure thrust term becomes a positive contributor to the thrust coefficient (P. Sutton). Due to this, the thrust coefficient at high NPR is maximised at larger divergence angles, as evidenced from the evidence set in Table 1. Alili's study tests multiple divergence angles across a range of high NPR values (89-1000), providing the most analytically complete picture of nozzle performance. Alili reports two optimum divergence half angles depending on the research objective: 15° for the greatest efficiency (highest thrust coefficient) and 23° for maximum raw thrust force generated. This distinction suits with the theoretical predication made in section 2: as the optimum angle shifts with each NPR value, no single angle can maximize performance at each operating condition. This implies that NPR & the optimum angle are considered to be a set of points that yield different values for C_T , for each range: Low, Intermediate & High. As the NPR value rises, the exit pressure climbs close to the ambient pressure and hence the NPR value approaches the ideally-expanded scenario, wherein NPR=Design value. Because of this, the pressure inside the nozzle doesn't need to be recompressed as the pressure gradient becomes small, leading to a reduction or weakening in the oblique shocks that formed before-hand (Papamoschou). Therefore, due to this effect, larger angles are favoured to maximize thrust coefficient at higher NPR values.

Similarly, Vargas' experimental study provides corroborating physical evidence to our set predictions as well – 1.57 lbf of thrust at 30° against 1.47 lbf at 15°, a 6.8% thrust advantage for the larger angle. This constitutes strong evidence that CFD systematically underestimates the true optimum for the given NPR. However, Vargas' experiment has structural methodological limitations as only 2 angles were tested: 15° & 30°. Furthermore, an exact value for the NPR wasn't specified. Given the limitations, both studies are directionally unambiguous — both identify larger angles at high NPR conditions — and this agreement between independent methodologies constitutes stronger evidence for the high-NPR preference for large angles than the agreement among three k-epsilon CFD studies at low NPR established earlier. To be precise, the high NPR evidence establishes a ceiling between 19° & 30° for the thrust optimized divergence half angle under near vacuum and high altitude conditions, which is substantially above the ceiling obtained for low NPRs

Across the evidence set, the thrust optimal divergence enable increases consistently with the NPR operating regime: from a ceiling constrained 13.5° at a low NPR of 9 through 15-25 across NPR values of 89-98, to 23° for maximum thrust in design conditions, and 30° experimentally in physical conditions. This showed us a variance of 20° across the optimum divergence angle for the NPR range tested (Dabir; Swaroopini; Hampali; Alili; Sudin; Vargas). The flow separation and internal shock formation threshold follows an identical trajectory as well — shock formation occurs at 13.6° at NPR 9 where severe over-expansion drives a strong adverse pressure gradient against the boundary layer, while at NPR 98 no internal shock formation is observed at angles as large as 23° — confirming that the optimal angle rose as NPR increased and over-expansion severity diminished (Dabir; Alili; Papamoschou et al.). Critically, this pattern is not visible within any individual study in the evidence set: Dabir observes only the low-NPR constraint, Alili observes only the high-NPR behaviour, and Vargas provides a single physical data point without theoretical framing. Hence, the progression only becomes visible when all studies are aligned on a common NPR axis, which is the function this synthesis performs (see Table 1). The pattern nonetheless carries a structural limitation of the transitional operating regime of NPR 25-89 being unstudied, meaning the exact NPR value at which the optimal angle crosses the 15° threshold cannot be determined from the existing evidence, and the rate of change of the optimal angle through the most dynamically active region of the ascent profile remains unknown. Despite this limitation, the directional consistency between the theoretical prediction established in Section 2 and the empirical pattern identified across the evidence set constitutes the central finding of this review: the thrust-optimal divergence half-angle in conical De Laval nozzles is a function of NPR, and not a fixed geometric constant (P. Sutton).

The operating regime, consisting of the Nozzle Pressure Ratio, is a primary explanation for the varying optimum divergence angles. However, the NPR values don't fully explain why Dabir got a higher optimum angle of 13.5° at a NPR lower than Swaroopini's. This highlights a striking anomaly in our trend-based study. The anomaly exists because both studies optimize their divergence half angles for different performance metrics. As seen in Table 1, Dabir explores the optimum angle through the lens of the thrust coefficient, which is also what we are reviewing, whereas Swaroopini's explores it through the lens of the Mach Number Optimization (Dabir, Swaroopini). Swaroopini's study optimizes for Mach number, which is similar to optimizing for Adiabatic efficiency in this context – how effectively does the nozzle convert the thermal energy (enthalpy) into kinetic energy (*Power Plant Lectures 4 Th Year Chapter 4: Nozzle*). This is a metric that captures the momentum thrust performance accurately but fails to account for the contribution of the pressure thrust term in the C_T equation. It is important to note that Mach Number is the ratio of the relative speed of the fluid to the speed of sound (NASA, "Mach Number"). At a lower NPR, the pressure thrust term becomes negligible and therefore maximizing for Mach number and thrust coefficient produce near-identical optimum angles. Another way to look at it is that, at a lower NPR, because shallower angles are favoured the correctional factor, λ, remains high, signifying that the loss in efficiency is small and mostly all the axial momentum contributes to forward thrust. However, at a higher NPR, like in the case of Swaroopini's, that operates at a relatively higher NPR than Dabir's, we can see that the metrics produce distinct optimum angles. A nozzle optimized for exit mach number favours a shallower angle while producing thrust force less efficiently due to increased frictional losses, whereas a nozzle optimized for the thrust coefficient favours larger divergence angles, that generates a greater pressure thrust but at a lower exit velocity, reducing the Mach number metric. This paper treats C_T as a performance metric as established in section 2, and treats the optimization of the Mach number as a different metric, rather than a contradiction to what is established earlier. Thus, the metric inconsistency is identified and weighted separately and is not used as a replacement to the primary correlation made earlier in section 2.

Therefore, a clean theoretical framework established for the optimum angle and the accounted disagreements of instances where the theory deviates from this behaviour have been presented above. However, another significant evidential limitation remains majorly unaddressed. With the exception of Vargas' study in 2013, all the other cases in the evidence set tend to rely on a singular computational practice of using CFD's k-epsilon models, which have limitations near the boundary of flow separation that have not been independently validated against against physical lab-tested measurements from this evidence set. This carries significant weightage as the separation constrained ceiling at a low NPR identified above occurs right below the point of flow separation, which is precisely the regime where the Reynolds-Averaged Navier-Stokes (RANS) formulation underlying k-epsilon modelling is theoretically the weakest. RANS closure via the k-epsilon model relies on the Boussinesq approximation, which covers an assumption that breaks down near separation points, causing k-epsilon models to predict separation onset at smaller angles than physical experiments observed (Wilcox). Given, these models consistently predict smaller angles than the physical reality, the sub-15°consensus may represent a modelling tendency rather than a physical optimum. This possibility is further substantiated through the superior optimum angle found by Vargas' study, an angle which no CFD study accurately reports. The question of whether the CFD-derived pattern reflects physical reality is therefore not a peripheral concern but a direct challenge to the reliability of the pattern's quantitative claims, and it is the precise question Section 4 will address by examining the specific mechanisms by which k-epsilon CFD models diverge from experimental results near flow-separation conditions. Thus, Section 4 will help us assess what the physical evidence implies about the true optimal angle range across the NPR spectrum.

CFD & EXPERIMENTAL LITERATURE

The aggregate trend established in Figure B conceals two patterns that become significant only on closer inspection, and together they motivate the analysis of this section. First, the empirical data sits systematically above the idealised theoretical curve across the full NPR range. Real life implications like the isentropic formulation, omission of viscous losses and real-gas effects, predicts the lower bound of the optimal angle rather than its realised value, and every category of study, computational and experimental alike, finds optima at or above this bound. Second, and more consequentially, the empirical points do not sit above the curve uniformly: at comparable NPR the experimental measurements consistently exceed the CFD predictions, with Vargas at 30° and NASA TN D-467 at 25° sitting well above Alili's computational optima of 15–23° at similar high pressure ratios. This example is not an anomaly, but rather a directional divergence between these two methodologies: the physical experiments locating the thrust-optimal angle higher than the simulations at matched conditions. The remainder of this section examines why this divergence arises, argues that it reflects systematic conservatism in the CFD methodology rather than genuine disagreement about the underlying physics, and establishes what it implies for the true position of the optimal-angle-versus-NPR relationship.

Case studies in the data set converge on the proportionate relationship between the Nozzle Pressure Ratio (NPR) and the optimum divergence angle in a CD Nozzle, and this has been established earlier in the paper as well. However, the case studies contain a majority of tests that are run on CFD K-epsilon models that severely underpredict the optimal divergence angle on the boundary of flow separation. Speaking of the methods by which the experiment is conducted, the only anomaly is the lab testing paper written by Vargas in 2013, which physically measured that significantly more thrust was produced at an angle of 30°, which represents a nearly 45% variance from Sudin, who tested for the same performance metric with CFD. These two bodies of evidence cannot both be considered true under an identical operation regime of high NPR, implying that either CFD is systematically underpredicting optimum angles or Vargas' experiments included variables that failed to be generalized into the existing pattern. Through this section we will examine which one of these situations have yielded these discrete outcomes and the approximate reasons for these.

As seen in Table 1, 5 out of 6 of our chosen case studies converge at the optimal divergence angle through CFD Analysis. Specifically, through RANS formulation with a k-epsilon closure. This highlights systematic conservatism when it comes to resolving for the optimum divergence angle. RANS is a widely used mathematical model used for turbulence modelling, which revolves around the averaging operation of the Navier Stokes Equation to obtain mean equations of turbulent fluid flows (Idealsimulations). The fundamentals of the modelling system stem from the Boussinesq eddy viscosity assumption (isotropic turbulence), which fails to resolve the complex, 3-D shockwave and boundary layer interactions which are inherent to highly underexpanded flows at high NPRs. RANS provides a time-averaged solution, whereas high NPR flow inherently features high-frequency pressure fluctuations and asymmetrical vortex shedding, that RANS systems fail to capture (Martelli et al.). Since a high NPR leads to a higher optimal divergence angle, tests of these angles cause extreme flow separation in the nozzle. Because of which RANS tends to predict earlier or later separation, completely missing the optimal angle that balances boundary layer growth and core expansion. An alternative, that helps engineers prevent the consequences faced by the inaccuracies of the model, was set to be the Shear Stress Transport (SST) Turbulence model. The model utilizes an advanced blending function that activates that activates the $k - \omega$model near walls and $k - \varepsilon$ in the freestream, along with a shear-stress limiter that prevents excessive turbulent viscosity in adverse pressure gradients. SST would be expected to predict separation onset at larger angles than k-epsilon, producing an accurate optimal angle (Könözsy). Critically, none of the CFD studies in the evidence set use SST or any higher-order turbulence mechanisms, which hampers credibility when it comes to examining the effect NPR has on the optimum divergence angle.

Beyond the turbulence model limitations examined above, a second, independent source of systematic conservatism exists in the geometric assumptions of both the RANS and SST CFD models. This limitation is observed in all 5 case studies that utilize CFD, and is a core limitation of CFD usage. All 5 studies employ 2D axisymmetric simulation, modelling the nozzle as a perfect revolution around its centreline and computing the flow in 2D. This assumption is valid for attached symmetric flow but fundamentally incompatible with the 3D asymmetric separation physics that govern nozzle fluid dynamics at high operating NPR regimes. At higher operating regimes, which theoretically require higher optimal divergence angles, the boundary layer detachment is no longer uniform across the nozzle's circumference: the separation initiates at one point on the nozzle and then propagates asymmetrically, generating adverse pressure gradients across the nozzle (Verma and Sankar). Coming to the CFD models, a 2D simulation cannot construct an asymmetric flow separation that originates at one place and then propagates throughout a nozzle. This is because the circumferential symmetry assumption forces any separation that occurs to be perfectly uniform around the nozzle exit simultaneously, a physical state that never occurs in real nozzles. This implies that 2D CFD either misrepresents the separation mode entirely or artificially delays separation onset because the symmetric mode is inherently more stable than the physical asymmetric mode (Verma and Sankar). The separation physics gets further complicated due to the transition between Free-Shock Separation (FSS) & Restricted Shock Separation (RSS), with each mode producing different pressure distributions and different optimal angle implications (Papamoschou). This transition is also crucial in all space flights as the NPR regime changes during ascent or throttling, which generates a sharp discontinuous spike in side load magnitude as the separation pattern distributes asymmetrically around the nozzle circumference. This is inherently unstable and three-dimensional, rendering it as invisible to the steady-state 2D axisymmetric RANS methodology employed across the entire CFD evidence set. Since the FSS-RSS transition governs the load environment at the separation boundary in all spacecraft nozzles, which limits the maximum viable divergence angle in reality, its absence from the CFD evidence set means that every optimal angle recommendation in Section 3 is derived from simulations that are blind to a consequential flow event at high divergence angles. This provides a second independent mechanism by which the CFD literature systematically underestimates the maximum possible angle.

The experimental evidence from Vargas' study from 2013, which is the only physically measured model in our data set and poses a direct challenge to the CFD consensus, also posseses similar methodological scrutiny as the computational studies critiqued above. It carries three very specific methodological limitations that restrict the study from refuting the optimum angle range obtained from the k-epsilon models of the CFD datasets. Firstly, Vargas' study examines only how two divergence angles affect the thrust force that is measured. Although it is established that there is a 6.8% increase in thrust force generated when transitioning from 15° to 30°, one cannot be sure of the movement of the trend between these two points, which reflects a key limitation of interpolation: assumed steadiness. Another important aspect neglected by testing at only two discrete angles is that the possibility of improvement in thrust performance beyond 30° is completely overruled. This leaves three distinct scenarios that the two-point experimental analysis cannot distinguish: that 30° is the true optimum, that the optimum lies between 15° and 30°, or that performance continues to improve beyond 30°. Second, Vargas's hybrid rocket propellant introduces a gas composition with a ratio of specific heats, γ, different from the air ($\gamma = 1.4$) used in the majority of CFD studies in the evidence set. A precise quantification is not possible from the reported data, but its direction can be estimated: hybrid propellants typically produce combustion gases with γ near 1.2, and since a lower γ raises the area ratio required to reach a given exit Mach number and lowers the exit pressure at a fixed area ratio, Vargas's nozzle would reach a different exit condition than an air-based nozzle of identical geometry (Ahmad et al.). The gamma discrepancy therefore remains an unresolved confound that prevents a precise NPR-matched comparison rather than a difference that can be corrected for analytically. Third, and the most critical bit for this paper's NPR framework, Vargas does not report the Nozzle Pressure Ratio at which the experiment was conducted. This means that the study cannot be precisely located on the theoretical optimal angle vs NPR curve established by the numerical analysis, and the comparison between Vargas's experimental result and the CFD studies remains approximate (Vargas). Collectively, these three limitations prevent Vargas from obtaining a precise optimum angle claim for a specific range of NPRs. However, these limitations do not undermine the directional significance established from this study: as the divergence angle increases to 30°, the increase in thrust generated plays a pivotal role in affecting the CT value and hence the optimal angle in the nozzle. This finding is consistent with the theoretical predictions made in Section 2, and hence serves as crucial supporting physical evidence.

Critically the limitations identified of the CFD RANS models, do not operate uniformly across all NPR Conditions: at low NPRs where separation onset occurs at small angles, within the reliable operating regime of k-epsilon models and where 2D symmetry is a reasonable approximation of the stable FSS separation mode, CFD results are likely to be physically accurate. However, at high NPR where the separation threshold is observed at large angles, wherein the boundary layer is operating in the adverse-pressure-gradient regime where k-epsilon fails, and where the FSS-RSS transition creates great instability (Wilcox), both limitations become simultaneously very severe. This is highlighted through Alili's case of 2024, wherein the 25° ceiling is the highest angle tested in the computation evidence set of this operating regime. This is registered as a physical optimum because of testing constraints of the k-epsilon model, thereby suggesting that rather than an optimal divergence angle, it is a computational upper bound which is obtained through restrictions of CFD modelling. Coming towards physical experimentation, Vargas' optimal angle of 30° proves the exact conservatism we notice when it comes to CFD models: physical experimentation consistently produces larger optimal angles than any CFD model can predict or test (Papamoschou).

CONCLUSION

As it stands, the primary finding obtained from this review converges at the fact that the thrust optimal divergence angle isn't a geometric constraint, but rather a function of the operating NPR regime, regardless of whether the method is computational or experimental. This was the hypothesis established in Section 1, theoretically predicted in section 2, critically validated in section 3 and extensively analyzed in section 4. The analytical result from section 2 clearly helped illustrate the relationship between operating NPR regime and the influence it has on the optimal divergence angle; the derivation showed that the size of the thrust coefficient evolves depending on the magnitude of $\frac{1}{NPR}$. Secondly, through the numerical computation in Figure A, we were able to quantify what the derivation provided directionally. Third, section 3 and Figure B, clearly showed the rising NPR figure, providing us with empirical validation over the full NPR range. Fourth, the methodological insight from Section 4, which suggested that the empirical optima sit systematically above the idealised curve, and experimental measurements sit above CFD at matched NPR, indicating the true optimal angle is higher than the conservative computational consensus.

To explore the solutions that are being raised by the questions in this review, heavy research is required in this single specific field that isn't present in existing literature. The research should extensively examine the relationship between NPR regime and the optimal divergence angle. It is pivotal for rocket scientists and aerospace engineers to conduct unified parametric investigations, spanning the full ascent range. This would trace the optimal angle trajectory as a continuous curve rather than as scattered-condition points. Furthermore, computational analysis should prioritize the employment of SST or Large Eddy Simulations over the existing k-epsilon models in CFD, which severely misrepresents separation onset at larger angles, as established in section 4 (Tanveer et al.). Computational geometry must be three-dimensional rather than 2D axis oriented, to capture the asymmetric separation as well as the hock separation transition dynamics that govern the viable-angle ceiling. And the computational results must be validated against physical thrust measurements at matched NPR, because the systematic offset between simulation and experiment identified in Figure B means neither method is self-sufficient. In the long run, the paper aims to be 'food for thought' for aviation research that could help in the formulation of cleaner and efficient systems that not only take into consideration geometric constraints, but also the operating environment of the propulsory system.

Collectively, the findings of the review help us establish a new lens through which rocket design can be examined and evaluated. It also aids in reconciling disagreements in existing literature by highlighting the multi-factorial nature of rocket design, one that heavily relies on the operating environment. Based on theory and the numerical computations, we were able to establish a directional trend that could aid the understanding of propulsion systems. Although we were able to establish directionality, quantification, in terms of why exactly all 14 data points lie systematically above the theoretical prediction, is also necessary to bring in greater accuracy in this field of study. Real-world effects like viscous boundary-layer losses, real-gas variation of the specific heat ratio at high temperature, and heat transfer through the walls, collectively shift the true optimal angle above the frictionless prediction. Notably, the analytical framework already accommodates one such correction: the divergence loss factor, λ , is itself a quantified adjustment, folding the momentum lost to non-axial exit flow into a single term within the thrust coefficient. The consistent offset in Figure B suggests that viscous and real-gas effects require the same treatment, that is a quantified correction factor, which is empirically calibrated and integrated into the analytical formulation. This would help raise the theoretical curve toward the observed optima. Developing such a factor represents a natural extension of this work, converting the idealised (theoretical) lower-bound curve into a predictive design tool. Lastly, the single most consequential question that remains open to this scientific field, is the transitional NPR 25-89 regime. It's the regime through which every rocket nozzle ascends and where the optimal angle shifts most rapidly, yet it remains unresolved by any study of sufficient methodological completeness, and that representation is the necessary next step towards a determined design relationship.

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