Actuation Lab

Rethinking Industrial Hardware.

Dragonfly Valve

Low Carbon Hydrogen Supply

HYS2154 Feasibility Assesment Report

26th of September 2022

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1. Glossary

Term	Definition
AM	Additively manufactured (3D printed)
ATEX	Two European Directives for controlling explosive atmospheres
Austenitic stainless steels	Stainless steel consisting mainly of face-centre-cubic crystal which is resistant to hydrogen embrittlement
BEIS	Department for Business, Energy & Industrial Strategy
BVAA	British Valve and Actuator Association
CAPEX	Capital Expenditure
CCUS	Carbon capture, utilisation and storage
CFD	Computational Fluid Dynamics
CO_2e	The amount of CO_2 which would have the equivalent global warming impact for any quantity and type of greenhouse gas over a 100-year period unless otherwise stated
Electrification	Powering by electricity
Electrolyser	An apparatus that produces hydrogen through a chemical process (electrolysis) capable of separating the hydrogen and oxygen molecules in water using electricity
Emission factor	The ratio between the amount of pollution generated and the output of the materials production process
EPA	Environmental Protection Agency
Ferrimagnetic	Body or substance with a high susceptibility to magnetisation
Ferrite	A ceramic compound consisting of a mixed oxide of iron and one or more other metals
GHG	Greenhouse gas
Green Hydrogen	Hydrogen generated by renewable energy
Grey Hydrogen	Hydrogen produced from fossil fuels
GWP	Global Warming Potential
HEE	Hydrogen Environmental Embrittlement
HEE index	An initial material screening tool to evaluate the severity of hydrogen embrittlement effects on certain materials
Hydraulic	Operated by liquid under pressure
Hydrogen embrittlement (HE)	Hydrogen embrittlement is a reduction in the ductility of a metal due to absorbed hydrogen
Net-Zero	A target of completely negating the amount of greenhouse gases produced by human activity by reducing emissions and implementing methods of absorbing carbon dioxide
NPL	National Physical Laboratory
PEM	Polymer Electrolyte Membrane
Pneumatic	Operated by air or gas under pressure
Pressure balanced	Gas pressure has no influence on the valve opening torque
SMR	Steam Methane Reforming
Stepper motor	A brushless electric motor that divides a rotation into steps
Torque	Rotational moment about an axis, Newton-metres (Nm)
TRL	Technology Readiness Level
USW	University of South Wales
WP	Work Package

2. Executive Summary

Low carbon hydrogen will be critical to decarbonisation and ensuring that the UK achieves its net-zero targets by 2050. Leaks and fugitive emissions from existing natural gas supply is known to be significant. Large scale hydrogen deployment will exacerbate this issue, due to the increased leak propensity of hydrogen. As hydrogen has been determined to be a potent greenhouse gas, with a global warming potential of 11 times carbon dioxide. The risks of ignition associated with hydrogen are also greater, leading to greater safety risks and a requirement for stricter leakage prevention. Valves, a critical part of any flow infrastructure, are major contributors to pipeline leaks, with most of this occurring around the valve stem.

Actuation Lab propose to develop a novel, stemless valve technology, the Dragonfly valve, to prevent the potential for these leaks and to enable net-zero hydrogen supply. The innovative Dragonfly mechanism requires very low torque to operate, and as such removes the need for a valve stem, the most common route for valve leakage, thereby ensuring zero-leakage over its lifetime by having no dynamic wear seals.

This project sought to validate the leakage issue with end-users, to verify that the valve mechanism was capable of stemless operation in target application conditions, to assess its compliance with regulatory standards, and to define a route to market including forming agreements for end-user trials.

The feasibility study and concept validation work undertaken have confirmed the technical, economic, and environmental feasibility of deploying the Dragonfly valve in hydrogen service, and that it will be capable of meeting the relevant standards and certifications required for this use.

Key findings in this study include:

- Hydrogen supply projects are in their infancy. Large valves are currently not required in most supply projects. Knowing this we have chosen to focus on developing Dragonfly valves with <4” diameter.
- Leakage is a notable concern for end-users, some of whom have set requirements that hydrogen systems not be placed in confined/indoor spaces due to explosion risks from potential leaks.
- Without intervention, increased leakage would mean total valve emissions will would only drop by 2.7% by implementing hydrogen in our network.

In addition to the benefits of deployment in hydrogen supply, the Dragonfly valve would be suitable for use across the whole hydrogen infrastructure in future, allowing for greater climate impact reduction and cost savings through further leakage prevention. Our estimates show that by 2050, up to 33 Mt CO_2e could be saved from leaking hydrogen valves every year by employing stemless valves in the supply chain.

3. Project Overview

3.1 Introduction

The aim of this project is to create the first valve designed specifically for hydrogen service and prevent large scale leakage across all gas networks.

The introduction of low carbon hydrogen will be critical in meeting the UK's legally binding commitment to achieve net zero by 2050. However, for this to be successfully achieved, significant technological developments need to be made at both system and subsystem/component levels to address leakage issues. Significant losses are already apparent in natural gas supply systems. Using the same natural gas components, qualified to the same standards, for hydrogen supply will undoubtedly lead to significantly increased leakage rates, due to the small size of hydrogen molecules and their ability to leak through paths where other gases would not. Combine this leakage with the fact that hydrogen itself is a powerful greenhouse gas (GHG) (11 times the impact of CO_2 over 100 years), its wide flammability range, and the high cost of hydrogen production, and it is clear that a strict policy to tackle all preventable leakage must be taken in the UK's future energy systems if net-zero and economic viability is to be achieved.

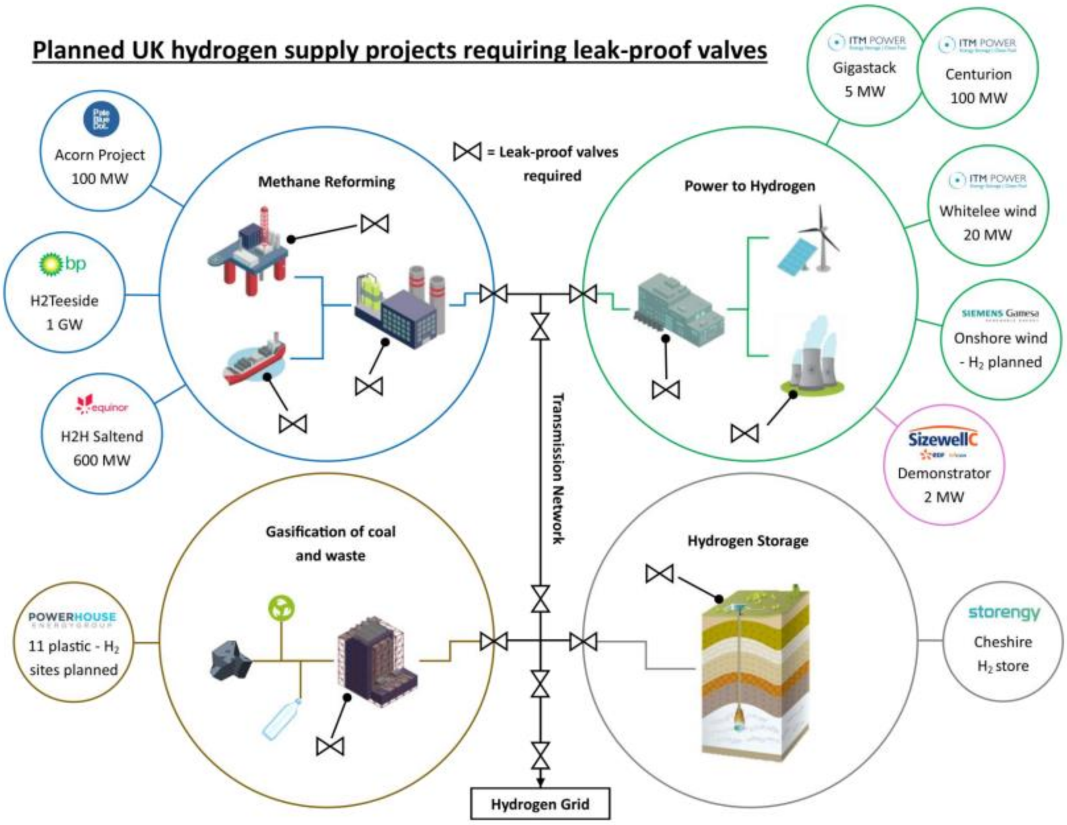


Figure 1: Hydrogen supply sites requiring leak free valves

Valves are an incredibly common component in any fluid system, and this holds particularly true in hydrogen supply systems, with valves being integrated right throughout these systems to control and isolate the flow of the gas (Figure 1). Unfortunately, valves are one of the main culprits of gas leakage from process equipment and pipelines, with most of this escaping from the valve stem; a shaft or rod protruding from inside the valve body to the outside world, which is connected to the moving element in the valve that is used to block the pipe. This stem is moved to open and close the valve and is either connected to a manual handle or to an actuator (pneumatic, electric, hydraulic etc), which operates the valve. As this stem provides a path from the inside to the outside of the valve, it represents a potential leak path for process gases, and as such is sealed using packing material (see Figure 2). This packing wears over time as the stem rotates against it, and therefore the potential for gas leakage increases as the valve cycles. Natural gas leakage from valve stems is currently a major environmental problem, with 59% of gas leakage from gas production equipment estimated to be coming from valves [1]. While regular maintenance and repair is recommended to reduce the scale of these stem leaks, extensive maintenance backlogs mean this frequently doesn't happen, and it has been shown that routine maintenance often does not solve the leakage problem, so full valve overhaul is required [2]. If this same valve technology is applied to the growing hydrogen supply chain, the rate of leakage will be significantly higher.

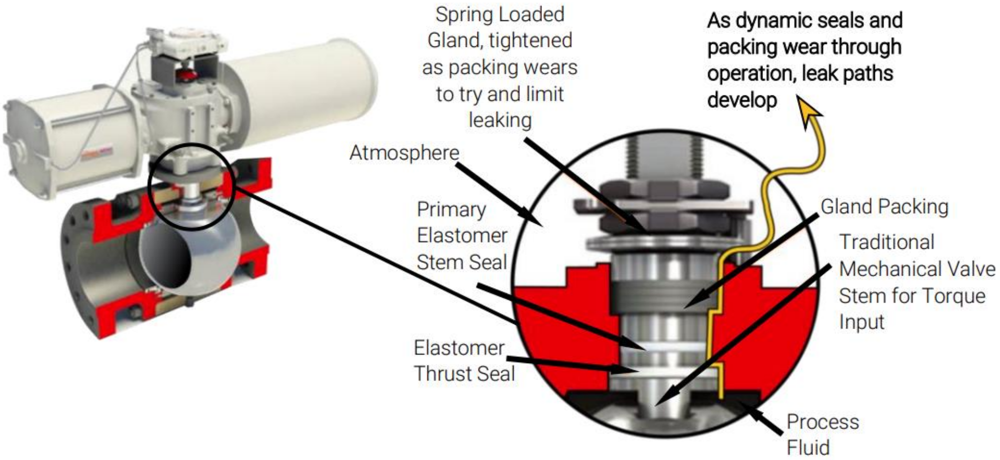


Figure 2: Traditional valve stem and sealing arrangement

Recognising these issues, Actuation Lab decided to develop a range of zero-emission valves, based on our proprietary "Dragonfly valve" mechanism. This design completely removes the traditional mechanical valve stem, replacing it with a non-contact, maintenance free, magnetic torque transmission through the wall of the valve, with the assembly sealed through a proven static seal (non-wear O-ring or gasket) or weld. Due to the relatively low torque potential of magnetic couplings, this requires a novel valve design which requires very low torque to operate. Frictional and pressure forces in typical valves make magnetic couplings non-viable, as it would require such a large coupling as to be impractical.

At the outset of this feasibility study, the Dragonfly had been developed to Technology Readiness Level (TRL) 4, in that a physical proof-of-concept had been built to demonstrate the working principles of the valve. The goal of this study was to determine the feasibility of developing this valve further in a follow-on demonstration project to TRL 8, from a technical, commercial, environmental, and economic perspective.

4. Results and Conclusions

4.1 Market Validation

While the issue of valve leakage is well known, the type, class, and sizes of valves in use in hydrogen production installations is not. To ensure that the development of the valve was focussed on the greatest market need, and to identify and quantify the size of the potential hydrogen leakage problem, Actuation Lab sought to engage with those working on hydrogen projects to determine if they would value a leak free valve, and secondly to ascertain their valve specifications. The goal was to establish the application, and therefore corresponding specification of the first valve(s) we will be developing and manufacturing.

During this market survey we documented conversations with around 30 stakeholders. The two key findings from this work can be summarised as follows:

1. **Emissions Concern.** The developing market is concerned about leakage from hydrogen valves, although much like methane leakage, it is poorly quantified, and its environmental impact not widely known. One operator revealed to us that they were **not allowing the use of hydrogen carrying valves in any internal spaces** due to the likelihood of stem leakage and the safety risk this would cause in an enclosed space.

2. **Equipment Sizing.** Current near-term planned low-carbon hydrogen projects are small, with small diameter pipes and valves. While we initially started this project looking for large valve applications (>4”) where the pressure-balanced low-torque features of the Dragonfly would have the most benefit, it’s now clear to us from our discussions with the market that a smaller valve (<4”) would be a better fit to the scale of green hydrogen projects that are currently in development. This led to a shift in our development focus to put a greater emphasis on a smaller Dragonfly valve mechanism.

4.2 Economic Feasibility (Product Costing)

Costings were developed for two variants of the Dragonfly valve; one for valve sizes over 4” and a simplified version designed for pipe under 4” that became our focus following market feedback on the size and requirements of valves on planned green hydrogen projects. Following an assessment of these costs it was decided to focus technical feasibility activities and demonstration phase planning on the updated smaller design in a range of sizes ranging from 3/8” to 4”. Future development of the larger Dragonfly design will take place when higher capacity hydrogen projects become more developed.

Detailed manufacturing cost estimates were carried out with comparison to competitor costs, both purchase and through life. In summary, for a ½” Dragonfly valve (the largest standard size available of current hydrogen compatible valves) we determined approximately 55% of the retail price of a traditionally stemmed hydrogen compatible valve. We believe this shows it to be feasible for the Dragonfly valve to be competitively priced particularly when combined with additional benefits and lifetime cost savings.

Considering the purchase, maintenance and repair costs associated with stem seals, and lost hydrogen through stem seal leakage, the predicted annual cost reduction was calculated to be roughly 135% of the purchase cost of an existing design per valve. Including indirect costs associated with energy usage and efficiency gains through electrification, the potential cost savings were calculated to be 240% of purchase cost, per year and per valve. Assuming a valve lifetime of 20 years (though many valves are left to operate long beyond this), this amounts to a total direct cost saving equivalent to 27 valve purchases, and 48 including indirect costs. This cost analysis assumes that:

- Hydrogen-service valves will be maintained and serviced at the same intervals as natural gas valves.
- Valve sizes and numbers used for future hydrogen supply can be assumed to be similar to those currently used in oil and gas supply and production.
- This valve is a new item in a new installation, as is likely the case with future electrolyser systems.

4.3 Technical Feasibility

4.3.1 Materials Compatibility

A range of materials were found that met the functional requirements for operation and which have been previously found not to degrade when exposed to hydrogen. All materials to be used in the design are equally applicable to use with natural gas and a host of other fluids for which unwanted leakage would have a significantly negative outcome such as CO_2 or ammonia.

Metals

The preferred metals for hydrogen systems are austenitic stainless steels to resist hydrogen embrittlement, with the standard metal from this group being 316L. Higher strength options include Nitronic 50, a nitrogen-strengthened austenitic stainless steel, and A-286, a NASA developed iron-based alloy, details of which are shown below.

Table 1: Appropriate non-magnetic and hydrogen safe materials, their allowable stress and price.

Material	ASME BPVC Allowable Stress (MPa)	Cost (£/m at required 90 mm diameter)
316L	115	436
Nitronic 50	230	1099
A-286	299	1173

Additively Manufactured Metals

In this feasibility project we have contracted HiETA Technologies to explore any additional risks associated with using Additive Manufacturing (AM) to produce metal components for a hydrogen valve. Additive manufacturing allows for intricate flow and noise controlling inserts to be manufactured and installed into the Dragonfly valve, that would not have been possible to manufacture using traditional methods.

It was concluded that AM 316L would be suitable for use in hydrogen service valves if certain control measures were put in place, and the material composition monitored.

Magnets

Through completion of a supply chain study and discussions with coupling manufacturers, it was determined that the use of magnetic couplings in hydrogen service will be feasible with appropriate material selection and protection methods.

4.3.2 Modelling Results

Valve modelling experts were engaged to verify the torque requirements for the smaller Dragonfly design, and to explore the influence of various geometric parameters on the all-important torque requirements that the magnet must supply. The model found that the minimum operating torque was approximately half that of an equal size, off-the-shelf valve.

The flow coefficient (Cv) is a critical performance index associated with the energy efficiency of any valve. We have utilised Computational Fluid Dynamics (CFD) to evaluate the flow characteristics of the Dragonfly valve and to determine the flow coefficient for varying valve open percentages. Flow coefficient performance comparisons of different competitor valves have been made in Table 2.

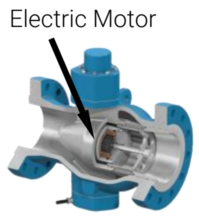
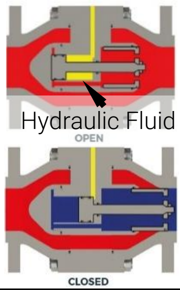
In this work we validated our CFD model by comparing our modelling results of a standard, commercially available, 1” valve to experimental results [3] which analysed and experimentally tested the flow rate of a 1” valve used in a thermal power plant. The model was then applied to the 1” Dragonfly valve to directly compare its performance and flow characteristics with flow in both directions.

A series of demonstrators were produced during the feasibility phase to explore manufacturability and assembly, test actuation concepts and validate the reduced torque.

4.3.3 Technical Competitor Analysis

The results show that the Dragonfly can achieve the low torque required for magnetic operation without compromising on flow capacity or having to employ complicated gearboxes within the valve body. The results show that the Dragonfly can achieve the low torque required for magnetic operation without compromising on flow capacity or having to employ complicated gearboxes within the valve body. Table 2 presents a technical comparison of what the results obtained in the feasibility study for torque and flow mean in comparison to both a traditional stemmed valve and other stemless valve competitors. The results show that the Dragonfly can achieve the low torque required for magnetic operation without compromising on flow capacity or having to employ complicated gearboxes within the valve body.

Table 2: Technical comparison of the Dragonfly valve to a traditional stemmed valve available in a hydrogen safe material and three stemless valve competitors. Note the method for removing the stem, the available valve size, flow capacity and operating force requirement.

Traditional Ball Valve in Hydrogen Safe Materials	Mokveld Zero Emissions Control Valve	Oxford Flow ES	Bighorn MagBall	Actuation Lab Dragonfly
				
Uses traditional mechanical valve stem and wear packing	No Stem through use of poorly accessible encapsulated motor within flow	No stem through use of hydraulic piston in centre of valve	No stem through use of complex gearbox in valve pressure body to increase magnet torque	No stem through smart torque reducing valve mechanism, allows magnet use without gearbox
Available up to 1/2" Size	Available over 6" Size	Available over 4" Size	Unknown	Initially Available up to 4" Size
High Flow	Low Flow	Low Flow	High Flow	High Flow
High Torque	Medium Torque	Medium Torque	Low Torque	Low Torque

4.4 Suitable Supply Chain and Manufacturing Partners

To ensure security of supply and scalability of the proposed technology, a supply chain study was completed, most notably covering the more unconventional elements of the technology such as the magnetic coupling.

4.4.1 Magnetic Couplings

The use of magnetic couplings is well established in industrial equipment that benefits from non-contact torque transmission allowing closed systems, thereby preventing a path for fluid and gas leakage. These couplings can also prevent vibrations being transmitted into the potentially delicate mechanisms inside equipment. The reduction in wear and the removal of expensive mechanical seals make these couplings virtually maintenance free. They are not typically used in valve operation due to high torque requirements, and where they are used, a gearbox is required on the internal side of the coupling. The Dragonfly valve requires low enough torque to be operated with such couplings. These couplings also need to be hydrogen compatible and ATEX compliant.

A suitable supplier was identified with the best combination of expertise, capabilities and size to perform development work for custom couplings moving forward. A three phase work proposal was formulated, in which this supplier would perform the first phase (baseline characterisation) during this feasibility study.

4.4.2 Automation Components

The original concept called for the development of our own automation system based on the use of ATEX certified stepper motors. The move to focus on smaller valve designs allowed for the use of standard 180-degree operation valve actuators, both electric and pneumatic. While this is beneficial, ATEX certified options tend to be much larger than required for our low torque valve. With the goal of a faster, more compact, lower torque electric actuator, we have begun discussions with an actuation developer to modify one of their solutions. Should customers require a pneumatic actuation system, a number of compact, ATEX compliant options are available off-the-shelf.

4.5 Regulatory Feasibility

We have engaged with a number of certification bodies on this project to understand if there were any fundamental issues that would prevent the valve being qualified for service. One of these contacts hosted our team during this feasibility study to carry out a workshop at a hydrogen gas test site. We have also received costed qualification plans from two organisations that are commonly employed as a valve certifying body, one of whom specialises in hydrogen testing. All believe the Dragonfly valve concept to be feasible from a regulatory and approval perspective.

4.6 Environmental Feasibility and Benefits

4.6.1 Reviewing the Scale of Current Valve Gas Leakage

The majority of gas leakage assessments of the gas industry have been carried out in the USA. These studies fall into equipment level measurements, which have been well summarised by Brandt *et al.* in 2016 [6] or using aerial analysis or satellite data. The most comprehensive equipment leakage survey of a complete gas supply network was that published by the US Environmental Protection Agency in 1996 [1]. The aim of the paper was to assess the leakage from valves, flanges, seals, and other connections to provide a bottom-up analysis of leakage in the US gas industry.

Table 3 gives a breakdown of key valve data we have been able to extract from this study. Valve leakage accounted for 13% of total gas lost through components, at 287,307 tonnes, or 8.05 million tonnes CO_2e. This was 5.11% of the total loss of methane to atmosphere from the gas supply chain.

Table 3: Valve gas leakage data from USA gas industry [6]

	Total valve leakage (tonnes)	Tonnes CO_2e/year	% of leaks from valves
USA gas production	206,148	5,772,146	59%
USA gas processing	26,776	749,735	5%
USA gas transmission	28,699	803,578	3%
USA gas storage	25,683	719,127	8%
Total US industrial gas supply (1992):	**287,307**	**8,044,586**	**13%**

Empirical evidence suggests that since the Environmental Protection Agency study, the leakage from equipment in the natural gas has not abated, and either the values obtained by the EPA were an underestimate, or leakage has increased. The 1992 study concluded that 1.4% of all the gas product in the industry was lost. However, a recent methane loss study by Alvarez *et al*. [4] estimated gas industry leakage levels to be 60% higher, at 2.3% or 13 million tonnes.

Since 1992, gas production in the US has doubled. Assuming US valve numbers scale to global numbers based on gas production volume, and valve emission factors of 20.74 m^3/year, a bottom-up estimate for valve emissions in the natural gas industry totals 71.5 million tonnes of CO_2e. Cumulatively, this would mean that 1.39 billion tonnes of CO_2e has been lost through valves over the last 20 years, as shown in Table 4.

Table 4: Extrapolated global valve gas leakage

	Total valve leakage (tonnes)	**Emissions (tonnes CO_2e/year)**	**Billion tonnes CO_2e since year 2000**	**% of gas leaks from valves**
Total Global industrial gas supply (2021):	2,552,844	71,479,639	1.39	13%

To approximate present day valve losses with a top-down method, Alvarez *et al.* [4] estimated that a total of 13 million tonnes of methane is lost to the atmosphere in the US every year. The US produces approximately 20% of the world's natural gas, so scaling this estimate according to global volume equates to losses of 65 million tonnes of methane, or 1.82 billion tonnes of CO_2e to the atmosphere every year from the global natural gas industry. In the EPA study [1], 5.11% of total methane loss was found to be through valves. Assuming a similar current ratio gives a current global estimated fugitive gas emissions from valves of 93 million tonnes CO_2e.

We have used data primarily from the USA to predict global leakage. There is little publicly available data on valve-specific leakage from UK assets; however we have worked with partners during the course of this study to verify leakage rates in the UK. Surveys carried out on UK gas processing sites have shown that over a third of total gas leakage is coming from valve stems. A leakage detection and repair survey carried out in 2020 on an offshore UK asset showed that similar levels of total methane leakage on the platform originated specifically from valve stems, equivalent to 638 tonnes CO2e/year. In extreme cases, valves were found to account for nearly 80% of leakage in similar surveys of upstream gas production facilities.

4.6.2 Predicting leakage from hydrogen valves

A recent top-down assessment of total hydrogen leakage from a future hydrogen grid was presented in a paper published by BEIS in April 2022 [8]. Their model estimates that a scenario in which approximately 23% of global energy consumption is supplied by hydrogen, replacing 40% of current fossil fuel energy, requires 859 Mt (Million Tonnes) of hydrogen to be produced every year. Current gas lost from the US gas grid is estimated at 2.3% of net product [4] and studies by the US Gas Transport

Institute indicate that hydrogen escapes 3x faster than natural gas [9]. In an analogous hydrogen supply chain, hydrogen escape could reasonably be assumed to be 6.9% of total hydrogen produced. This would equate to 59.3 million tonnes of hydrogen. Assuming hydrogen's global warming potential is 11x CO_2 over 100 years, its global warming potential would equal 652 million tonnes CO_2e. If 5.11% of total leakage originated from valves as measured in the EPA study [1], total H_2 fugitive emissions due to valves in this scenario would total 33.3 million tonnes CO_2e each year.

To examine leakage at a component level, with hydrogen leaking 3 times faster by volume than natural gas (at the same pressure), the use of similar valves would result in average valve emission increasing from 20.74 m3 /year when carrying methane, to 62.2 m3 /year, or 5.1 kg/year with hydrogen. Using a GWP of 11, this is 51.6 kg CO2e/year per valve [1]. The 859 million tonnes of hydrogen predicted to be produced in 2050 equates to 10.48 trillion cubic metres of gas at standard temperature and pressure. By scaling estimated hydrogen valve emissions by the number of valves required to handle this volume of gas, the total hydrogen leakage would total 25 million tonnes CO2e globally.

4.6.3 Accounting for methane valves and leakage distribution

Currently, 95% of hydrogen is produced through Steam Methane Reforming (SMR), which uses an estimated 165.3 Mt of methane as a feedstock. This methane is extracted by the established Oil and Gas industry in which significant leakages occur, as described in Section 4. If we assume that 2.3% of that methane is lost in production, and 5.11% of this is lost from valves, annual valve-related emissions in SMR operations are currently 199,000 tonnes of CH4 which equates to 5.57 million tonnes CO2e with a GWP of 28x CO2.

Brant *et al* [6] showed that 5% of all valve leaks in US gas infrastructure were responsible for 79% of valve emissions. In the leakage study carried out our partners on gas processing stations, 5% of valves were responsible for 47% of leakage. Replacing these worst offending valves in the natural gas supply chain with a leak free alternative is likely to eliminate at least half of upstream SMR related valve emissions, or 2.79 million tonnes CO_2e. The hydrogen for net zero report [11] released by the hydrogen council in 2021 estimates that in 2050, around 30% of hydrogen will be produced as “blue hydrogen” using SMR and CCUS. Should this be the case, 537 Mt of CH_4 would be required as a feedstock. With no change in valve technology, this would result in 17.67 Mt of valve emissions in 2050.

Table 5: Estimated valve methane emissions for SMR and global energy in 2021 and 2050.

		2021	2050
Methane for SMR	Total valve emissions ($MtCO_2e$/year)	5.57	17.67
	Reduction replacing worst 5% ($MtCO_2e$/year)	2.79	8.84
	Lost product saving (£)	£46,978,467	£149,105,904
Methane for global energy	Total valve emissions ($MtCO_2e$/year)	93.00	60.45
	Reduction replacing worst 5% ($MtCO_2e$/year)	46.50	30.23
	Lost product saving (£)	£784,687,500	£510,046,875

Using the same assumptions and based on our estimates that 93 Mt CO_2e is currently lost from valves in the natural gas industry, replacing the top 5% worst offending valves across the whole natural gas industry could eliminate 46.5 Mt CO_2e. Imperial College London released a paper in 2021 which estimated that the natural gas industry would have to shrink by 35% by 2050 to reach our Net Zero targets [12]. Assuming leakage would scale accordingly, methane valve leakage could total 60.45 Mt CO_2e in 2050 with no innovation, with 30.23 Mt CO_2e coming from the worst 5% of valve leaks. Table 5 summarises the methane related emissions from valves for SMR methane and generally, as well as the cost of this leakage in lost product.

It is clear that methane leakage from valves is still going to be a significant environmental burden as the hydrogen industry scales if action is not taken and will likely continue to exceed those of hydrogen even with a 35% reduction in extraction. The graph below illustrates this and shows that although methane related valve emissions will reduce, the corresponding increase in hydrogen leakage would mean total valve emissions will would only drop by 2.7%.

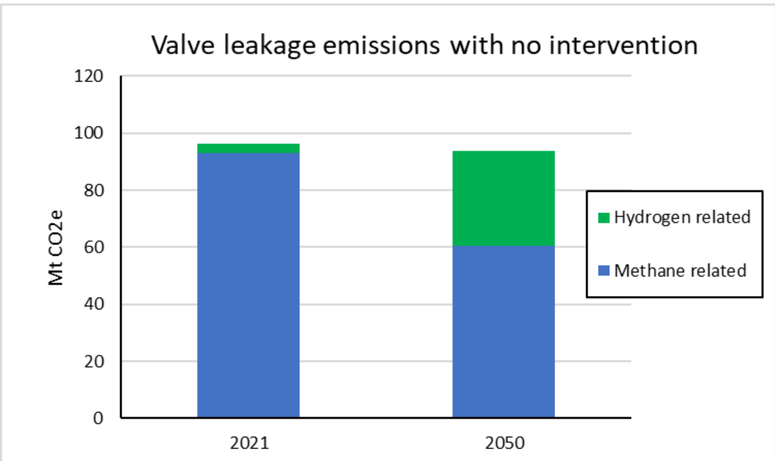


Figure 3: Predicted impact of valve leakage emissions of no intervention is undertaken

Summary

With the various scenarios considered, hydrogen leakage from valves will have significant climate impacts, with our estimates of between 25 - 33.3 million tonnes of CO_2e leaked from valves in a future hydrogen grid, the latter being equivalent to New

Zealand's total annual emissions. Methane leakage from valves in 2050 is likely to still exceed emissions from hydrogen valve leakage. In order to have the biggest climate impact, our commercialisation plan must be to concurrently target the methane valve replacement market, both inside and outside of the hydrogen supply market.

4.7 Preventing Valve Leakage for Safety

The flammability and explosive characteristics of hydrogen are distinctly different from hydrocarbon fuels such as methane. While hydrogen has a similar lower explosive concentration limit, it has a much higher upper limit [13]. Hydrogen is also around 3.5 times more buoyant than methane, meaning hydrogen disperses and dilutes more rapidly. In an open environment, a hydrogen leak is likely to disperse rapidly, however, in enclosed spaces hydrogen will accumulate, particularly in overhead pockets. Overhead blocks and enclosures can allow hydrogen to build to dangerous concentrations. Hydrogen has a very low minimum ignition energy; this means that it is often difficult to determine the exact mechanism and cause of an ignition when it occurs [11]. Early inclusion of hydrogen in UK energy networks involved blending hydrogen with natural gas, at concentrations of up to 20%. At these concentrations, there is little change to any associated risk factors [12]. However, in experimental research by Lowesmith et al [13], conducting large-scale explosions showed that by adding 50% hydrogen to the blend and simulating a gas leak, a significant increase in explosion flame speed and overpressure was observed. The H21 study showed that the use of pure hydrogen in gas infrastructure is calculated to increase the Potential Loss of Life estimates by a substantial percentage in the unrealistic scenario that equivalent components and controls as for Natural Gas are used.

A number of reports and programmes have been carried out to assess how to safely incorporate hydrogen into our networks. An example is EC funded HySafe, "InsHyde - Hydrogen Releases in Confined and Partially Confined Spaces". This has shown that the use of hydrogen requires additional detection and ventilation systems as compared to natural gas, and that additional fire and explosion safety requirements will be needed to prevent accumulation and potential explosion/detonation.

Another program run by the US Department of Energy has collated data and reports relating to incidents occurring that involve hydrogen (H2 Tools). A number of safety incidents have taken place due to hydrogen leaks, some specifically from valve stems [17] [18] [19], at least one of which resulted in an ignition [20]. The Dragonfly valve avoids any issue from stem related failure, thereby significantly reducing the risk of injury and damage to property.

We consulted with several hydrogen users, all of whom cited concerns about safety issues surrounding valve leakage that could occur as projects scale. One operator specifically outlined that they were not allowing the use of hydrogen carrying valves in any internal spaces due to the likelihood of stem leakage and the safety risk this would cause. The average methane leak from valves measured in the studies summarised by Brandt et al [4] was 2.15 m3 /hour, and maximum of 264 m3 /hour. The same valves carrying hydrogen would have a mean leakage rate of approximately 6.45 m3 /hour and a maximum of 793 m^3/hour, posing a serious explosion risk in enclosed or covered spaces.

5. Demonstration Project Description

The goal of the Phase 2 demonstration project is to develop the Dragonfly valve from its current TRL4 to TRL8, which involves proving the technology works through testing and qualification in a commercial design. To achieve this goal, the valve concept will required design and verification work to be carried out, along with prototype manufacture and assembly. Subsequently, prototype units will be functionally tested and qualified to appropriate standards by appropriate testing bodies to ensure they are safe and suitable for use in hydrogen production and supply systems. Finally, the approved valves will be trialled for 6 months on a bespoke flow loop, representative of conditions in a commercially available electrolyser. As valves are ubiquitous throughout gas flow industries, this technology is important in enabling a hydrogen economy across all its sectors. The project is set to span 23 months and is broken down into 6 work packages as follows.

5.1 WP1 Project Management, Stakeholder Engagement and Reporting

This involves all project management activities, quarterly meetings with an advisory panel of project stakeholders and reporting of project outcomes. The aim of this work package is to ensure that the project is managed successfully, and that the stated objectives are achieved.

5.2 WP2 Business Development

This work package will include tradeshow attendance, conference presentations, customer engagement to secure future trials and sale opportunities, as well as engagement with potential distributers and licensees of the technology. Securing such agreements will be key outputs for this demonstration phase of the project, and will accelerate our route to market.

5.3 WP3 Engineering Design and Verification

This work package is largely concerned with expanding the range of valve sizes to be demonstrated on this project, and subsequently sold following certification. Outsourced verification work is to be conducted to ensure the valve meets pressure body integrity requirements in line with ASME BPVC Sec VIII Dev 2. The work package will also see design for the hydrogen safe magnetic couplings undertaken. The work package will output drawings and required files to progress to the prototype manufacturing stage. This work package is expected to span the first 6 months of the project.

5.4 WP4 Manufacture and Assembly

This work package will involve the sourcing of all off-the-shelf components, and contract manufacturing of all test articles required for certification, qualification, and demonstration. All test articles are expected to be delivered and assembled by February 2024.

5.5 WP5 Test, Certification and Qualification

Test and certification are critical parts of qualifying new safety critical equipment like the Dragonfly Valve. This will first involve inhouse testing of novel elements that include the bearings and seating arrangement. This will be followed by third party testing to qualify the valves, both for sales, and to deem them safe for demonstration deployment. This testing and certification will include:

Such testing is carried out externally due to the requirements for witnessing by notified bodies for certification, and due to the large capital expenditure required for the facilities needed to conduct these tests.

Physical testing will begin internally in August 2023. External testing will begin in February 2024, and is to be completed by June 2024.

5.6 WP6 Demonstration

Our partners, University of South Wales (USW) will be demonstrating the valve over the course of 6-months. This demonstration will follow the completion of the physical testing programme carried out in WP5, to ensure that the valve has been proven fit for purpose and thereby minimising the risk of early trial unit failure. The University of South Wales will design a flow loop, specify and procure equipment, and ultimately build and house the flow loop. Flow loop design will begin at project kick-off, to allow sufficient time for fabrication (starting September 2023) and commissioning (starting May 2024) to be carried out. The 6 month trial programme will then commence in July 2024.

6. Demonstration Design

For demonstration of the Dragonfly valves, we will be integrating 3 valves (3/8”, 1” and 2” in size) into a hydrogen flow loop (Figure 4), representative of process conditions in a hydrogen electrolyser. The flow loop will be designed and operated by partners at the University of South Wales Hydrogen Centre, led by Dr Jon Maddy. Pressurised, gaseous hydrogen will flow around the loop and through the valves, which will be cycled open and close repeatedly, to mimic the conditions they will experience in future hydrogen supply service.

As outlined in Section 5, the flow loop design will commence at project kick-off, which will be carried out by USW. This design phase will take 6 months, and will be followed by an 8 month fabrication phase, wherein the flow loop will be assembled. Subsequently, 2 months of commissioning will be carried out, after which the loop will be ready to host Dragonfly valve units for 6months following the certification testing program.

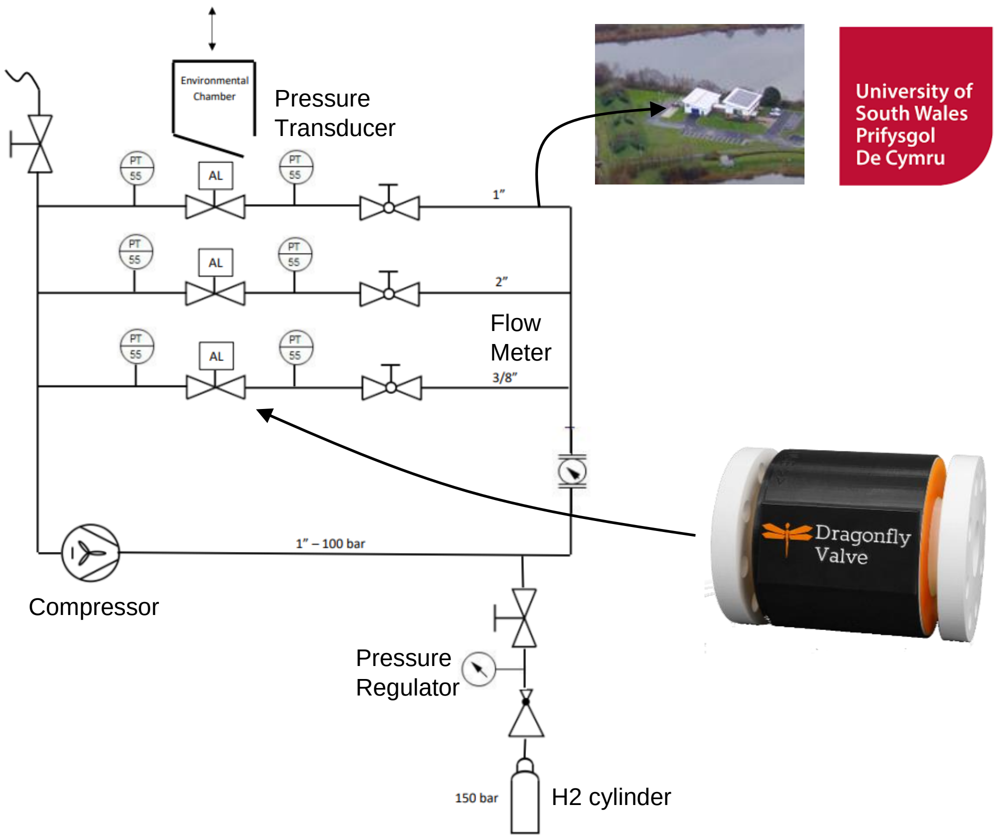


Figure 4: Demonstration setup

The demonstration program will subject the valves to accelerated lifetime testing in worst-case operating conditions, meaning that the valves will be subjected to extreme conditions to determine their expected reliability over a 20 year lifetime, whilst only requiring a 6 month testing period. The system will be capable of pressures of 100 bar, with a max differential pressure across the valves of 80 bar. The flow loop will be equipped with instrumentation to monitor the condition and performance of the valves online, including in-line pressure transducers, temperature monitoring, and acoustic emissions detection. Environmental chambers will be used to subject the valves to the full range of expected operating conditions.

7. Costed Development Plan

The development plan for the demonstration phase has been costed at £2.8M, and will include the manufacture of 100 Dragonfly valves to be used in test, certification, and demonstration activities. Some of these valves will be optimised for control applications and contain additively manufactured flow inserts, for better flow performance and noise abatement. The manufacture of this ambitious array of test articles, including all required automation and instrumentation to complete the test program has been costed through a range of manufacturers and component suppliers.

The demonstration project is estimated to entail: labour costs between £980k - £1,198k, with associated overheads between £196k - £239k. Material costs are anticipated to range between £750k - £880k, sub-contracting costs range between

£416k - £541k, and travel costs between £84k - £90k. Other costs, primarily associated with software licenses, training and PPE, contribute £95k - £108k.

Design activities on Phase 2 are limited to verification simulations to confirm product safety and performance prior to manufacture, the expansion of the size range of designed valves, and completion of design-for-manufacture. Design verification work will be undertaken by specialist valve simulation sub-contractor, while another subcontractor will be employed to complete the custom magnetic coupling development.

The bulk of subcontracted work will be applied to performing physical testing by specialist valve test houses and the issuing of qualification. Qualification certificates can only be issued by third party notifying bodies; thus, this is an external cost that cannot be avoided.

Business development activities are aimed at supporting the commercial development of the product beyond the end of the pilot. We aim to attend 10 tradeshows throughout the Phase 2 project, exhibiting at 6 of these. Travel is also included to support meetings that could facilitate manufacturing, distribution and licensing deals.

8. Rollout Potential

Within the hydrogen supply industry

The table below gives an indication of where valves are used in the hydrogen supply industry and the scale of number of valves at each site. SMR, methane extraction and distribution are replacement markets for our valve, whereas most of the green hydrogen production and storage sites will be new-build and rapidly growing markets.

Equipment	Valves/site	Scale	Notes
Electrolysers	100 – 1,000	Europe's largest electrolyser could manufacture 1,300 tonnes H_2/year. 660,000 of these would be required to meet 2050 demand.	A typical 50kW PEM electrolyser has 94 valves (data from USW). Whilst this number won't scale linearly with capacity, a multi-mega Watt electrolyser site could utilise over 1,000 valves.
SMR Plants	100 – 10,000	95% of hydrogen production produced via this method. A large SMR such as Air Liquide's SMR-X will produce 4,000 tonnes H_2 a year and house over 1,000 valves.	Significant replacement market. May decline as green hydrogen increases if CCUS not optimised.
SMR associated CH_4 extraction	1,000 – 2,000+	CH_4 extraction will continue into the foreseeable future and feed SMR processes. There are over 500 offshore platforms in the North Sea alone [21].	Number of valves based on EPA data for US offshore platforms. Methane leakage will be prevented in this instance, we would target 5% of valves which emit 47% of methane gas.
Alternative H_2 production	TBC	TBC	Multiple technologies being developed as part of the BEIS hydrogen supply competition.
Storage	Up to 2,000	Hydrogen storage ranges from small tanks to underground salt cavern storage.	Number of valves/sites based on the average from EPA data on gas storage sites in the USA

Transmission	1000's	Hydrogen is a key focus area for the National Grid [22]. Current network has 4,760 miles of pipeline and 618 above ground installations.	Transmission valves are typically large bore, and would require our 4"+ design, which will be developed after the <4" design

Decarbonisation opportunities in adjacent applications

As part of this project, we are developing the Dragonfly valve for general hydrogen use, which means it will be applicable in the broader hydrogen economy, not just supply. By successfully developing a hydrogen-ready Dragonfly valve for the hydrogen supply chain as part of the Low Carbon Hydrogen Supply 2 competition, we will be able to support the safe and sustainable development of hardware allowing the decarbonisation of steel production and aviation. Doing so could eliminate over 10% of the world's CO_2 emissions.

9. Route to Market Assessment and Impact

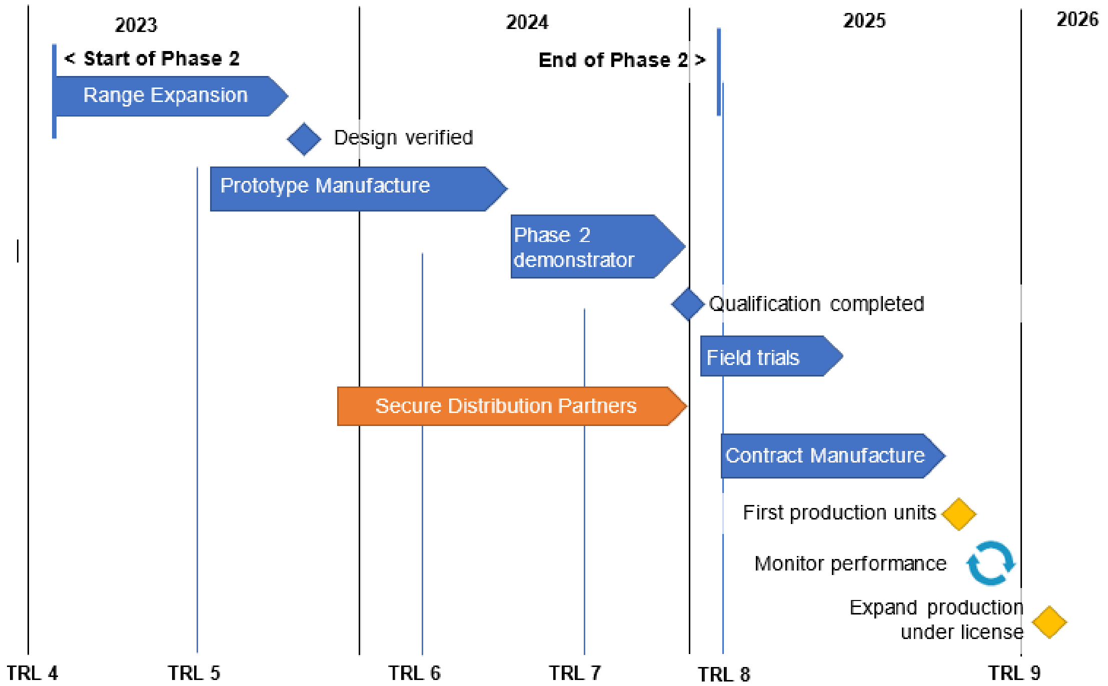


Figure 5: Key steps to take the Dragonfly valve to market

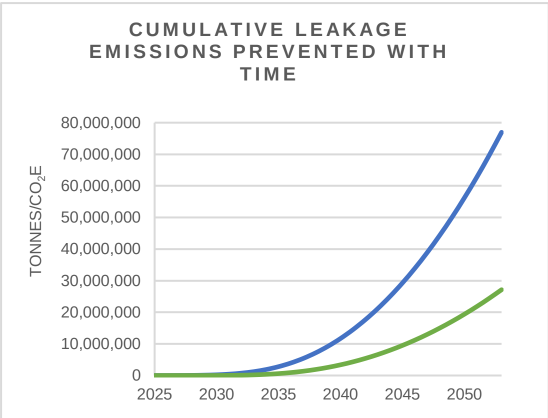
Figure 5 shows the route to market we aim to take. Following development of the 3/8"- 4" hydrogen gas valve, primarily aimed at green electrolyser applications, we will expand the range by, for example, developing cryogenic versions certified for use in green aviation, or large valves for nuclear energy.

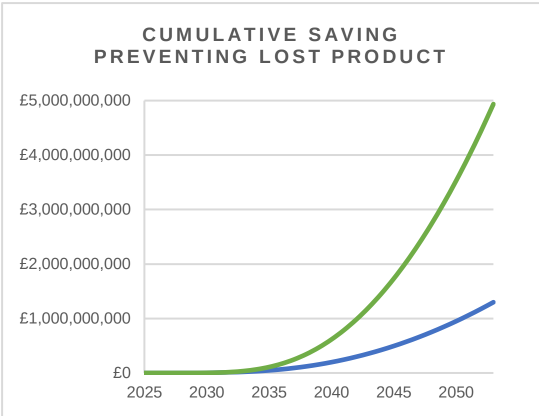
Having created two new full-time roles in Phase 1, we intend to employ a further 7 roles as a direct result of this Phase 2 funding, and the project will underpin growth of the company and our emerging UK supply chain.

9.1 Projected Valve Sales and Resulting Environmental Benefit

We have modelled a scenario of valve roll-out into the hydrogen and natural gas market over the next 30 years and the associated environmental benefit. There are still significant uncertainties around the size of the future hydrogen market, how quickly it will scale, by how much natural gas extraction will decline and the number of valves that will actually be required. This illustrative example provides a view to the potential impact of our technology in comparative natural gas and hydrogen applications.

These leakage numbers are only from gas leakage prevented from valves in the supply chain. It does not consider the emissions savings due to projects that are facilitated because of the adoption of our technology, gas use or adjacent markets. The emission factors used in these estimates are the average values derived for valves in gas supply. For methane in particular, much larger emission savings are achievable if the leakiest 5% of valves are replaced with our technology.





9.1.1 Valve Sales Beyond our Hydrogen Supply Scenario

There is significant potential to roll-out the Dragonfly valve into the adjacent markets beyond the hydrogen supply chain. Our study focussed on utilising our valves for hydrogen supply for use as energy. However, it is estimated that over 50 Mt of hydrogen will be required to replace coal in the steel manufacturing process. Our valves will be directly applicable in hydrogen production and storage in the steel industry, supporting an 8% reduction in global greenhouse gas emissions, so will be another market we can target concurrently. The other large opportunity to facilitate emissions reduction with our technology is by enabling leak-free valves for hydrogen aircraft. We will build upon the technology demonstrated in Phase 2 to create an aerospace grade Dragonfly valve, which would help facilitate a 2.4% reduction in global CO_2 emissions [23] through use of hydrogen as a fuel.

10. Summary of Benefits and Barriers

10.1 Benefits to industry

10.1.1 Safety

Will ensure the safety of future hydrogen projects with enclosed spaces, enabling the increase in project size without an increased risk of explosion.

10.1.2 Environmental benefit

By developing the Dragonfly valve with the hydrogen industry, we can prevent the same fugitive emission crisis from occurring in hydrogen systems as in the natural gas industry. Total preventable valve leakage in 2050 from hydrogen supply valves is estimated to be 24 – 33 Mt of CO_2e/year. The same Dragonfly technology can be deployed in the natural gas industry, where valve emissions currently total between 71 – 93 Mt of CO_2e/year.

Indirectly, utilising the Dragonfly valve will facilitate the use of hydrogen in enclosed spaces where it was not previously possible. This will assist in making it possible to safely utilise hydrogen in sectors such as aerospace and shipping, which currently contribute to 10% of the world's emissions by burning traditional fuels.

10.1.3 Prevention of lost product

All fugitive emissions represent lost product. In our "roll-out" scenario presented in this study, our technology will be preventing half a billion pounds in lost hydrogen product every year in 2050.

10.1.4 Reduction in servicing costs

Due to reduction in required valve servicing, an annual direct cost reduction of £400 per valve purchased may be achieved. Indirectly, energy savings due to electrification of valves compared to traditional pneumatics total 135% of the purchase cost of a traditionally stemmed hydrogen compatible valve per year, per valve. Assuming a valve lifetime of 20 years, a total direct cost saving equivalent to 27 such valve purchases per valve, and 48 including indirect costs, is achievable.

10.2 Barriers and Risks

10.2.1 Financial

Actuation Lab is not yet generating revenue from product sales or licencing, presenting a financial risk. The company relies on a combination of grants, R&D contracts, and private investment. If awarded Phase 2 funding, Actuation Lab will claim funding from BEIS to allow development of the Dragonfly valve. To support cashflow, and valve development for adjacent applications, the company set out to raise private funding this year. To support scaling of sales beyond the hydrogen supply competition will require further private investment in the company in early 2025. We will begin the fundraising process in 2024 and explore the possibility of raising funds from a strategic corporate investor in our industry.

10.2.2 Commercial

It has become clear that to mitigate against supply chain delays and ensure quality, we must utilise UK and European manufacturers for manufacture of subcomponents of our valves in Phase 2 and beyond.

A key component of our valve design is the magnetic couplings, where traceability of the source of rare earth metals and security of supply cannot always be guaranteed. During Phase 1 we found and began working with a US Department of Defence approved supplier, who we are confident can guarantee security of supply to UK companies. In future we will look to develop alternate magnetic solutions, including the use of very low-cost ferromagnetic internal couplings, and emerging low-cost, yet high strength magnetic materials.

New technology can be met with resistance to adoption by appearing radical, particularly in the valve market. We are mitigating against this by seeking to licence our technology through established manufacturers and working with the supply chain during our Phase 2 project.

10.2.3 Technical

The unique Dragonfly valve mechanism relies on elements that are not common to traditional valve design. Although careful selection suggests these elements should be able to provide the lifetime and performance that is required, this has not yet been tested in a simulated or real environment. This is to be mitigated against by carrying out material level testing with external manufacturers, and full system testing internally within the first 6 months of the demonstration phase project, to allow time for material changes and design modification if necessary.

10.2.4 Certification

Due to its intended application in hydrogen service, the valve will need to be approved for use in explosive atmospheres. This approval in general aims to ensure that any equipment used is not capable of generating an ignition source (i.e. a spark or high temperature surface). Some elements of the Dragonfly valve differentiate it from other valves, and as such the risks associated with completing this approval are higher. To mitigate against this, a design review will be held within the first 3 months of the project with the notified body chosen for our approval plan, in order to assess any potential ignition risks and to develop a testing plan to reduce any determined risks.

10.2.5 Resource

A barrier to rapidly scaling sales and licencing technology are access to facilities and highly skilled personnel. We have sought suitable premises and developed a robust hiring strategy and have begun seeking key hires for the next stage of development.

11. Dissemination

As well as many stakeholder meetings, the following dissemination activities have been undertaken during the feasibility phase:

- Attendance at BVAA spring conference and displaying the Dragonfly valve at their desktop exhibition (Atkins, Bristol)
- Becoming members of NOF and engaging with other gas supply members.
- A one-day workshop hosted at a hydrogen test facility, attended by staff of gas distribution networks and members of the Institute of Gas Engineers and Managers.
- Exhibiting the Dragonfly demonstrator at the SetSquared TechXpo to a range of investors.
- A workshop session at potential licensee's premises to present the Dragonfly concept to their engineering team and gain feedback on manufacturability.
- A hands-on development day with a valve integrator to experience issues with current valve and actuator designs, and to tour and present the Dragonfly concept to different groups within the business.

12. Conclusions

Phase 1 of this project has concluded that the development of the leak-free Dragonfly valve for hydrogen supply operations is both feasible and necessary.

It has been found that there is a clear market need and desire for the Dragonfly valve, with hydrogen users concerned about the likelihood of hydrogen leaks from valves stems and resulting, economic, environmental and safety issues that will result from this. It was also concluded from market engagement that the first range of Dragonfly valves should be relatively small in diameter (3/8" to 4") to best match the needs of currently planned green hydrogen projects.

The technical feasibility of the Dragonfly for hydrogen (and other gases) was confirmed, with suitable materials selected, torque requirements determined, and flow capacity verified. Areas of criticality were established, with specialist supply chain partners engaged with and plans developed for testing these areas in Phase 2. Wider certification and qualification plans were also created. This feasibility work has allowed for a Phase 2 demonstration project to be planned and costed. This follow-on work will span 23 months and cost £2.8M, concluding with the demonstration of the Dragonfly valve by the University of South Wales.

This feasibility work also allowed the need for a leak free hydrogen valve to be established. It was determined that up to 33 million tonnes of CO_2e a year could be leaking from valves in 2050, equivalent to New Zealand's total annual emissions if outdated existing valve technology is to continue being used. Add to this environmental impact the continued leakage of methane, the safety risk of highly flammable hydrogen and the cost of lost product, and it becomes clear that we must develop better valve designs to support the supply of hydrogen in a net-zero future.

13. References

[1] National Risk Management Research Laboratory, “Methane Emissions from the Natural Gas Industry, Volume 8: Equipment Leaks,” Environmental Protection Agency, New York, 1996.

[2] K. Sotoodeh, “Why packing adjustment cannot stop leakage: Case study of a ball valve failing to seal after packing adjustment during fugitive emission as per ISO 15848–1,” in *Engineering Failure Analysis*, vol. 130, 2021.

[3] C.-W. Y. C.-S. &. L. C.-W. Kang, “Experiment and Flow Analysis of the Flow Coefficient Cv of a 1 inch Ball Valve for a Thermal Power Plant,” *Journal of the Korean Society of Manufacturing Process Engineers,* vol. 3, 2019.

[4] R. A. Alvarez, “Assessment of Methane Emissions from the U.S. Oil and Gas Supply Chain,” *Science,* pp. 186 - 188, 2018.

[5] D. J. Zimmerle, “Methane Emissions from the Natural Gas Transmission and Storage System in the United States,” *Environmental Science & Technology,* pp. 9374-9383, 2015.

[6] A. R. Brandt, “Methane leaks from natural gas systems follow extreme distributions, impacting gas sustainabilty,” *Environmental Science and Technology ,* vol. 50 , no. 22, p. 12512–12520, 2016.

[7] American Gas Association, “Natural gas reserves and producing gas wells,” American Gas Association, 2021.

[8] N. Warwick, “Atmospheric implications of increased hydrogen use,” UK Government, London, 2022.

[9] NREL, “Blending Hydrogen into Natural Gas Pipeline Networks: Key Issues Review,” National Renewable Energy Laboratory , 2013.

[10] Gas Turbine World, “Green Hydrogen powering gas turbines: realistic strategy?,” 2022.

[11] Recharge News, “Energy Transition,” 2021.

[12] C. Brogan, “Use of natural gas will decline if we are to achieve 1.5°C climate targets,” 2021.

[13] ARUP, “Five Minute Guide to Hydrogen,” [Online]. Available: https://www.arup.com/perspectives/publications/promotional-materials/section/five-minute-guide-to-hydrogen.

[14] L. d. Broisia, “HySafe,” [Online]. Available: http://www.hysafe.org/download/1042.

[15] H21, "H21 PHASE 1 TECHNICAL SUMMARY REPORT," 2021.

[16] B. Lowesmith, C. Mumby, G. Hankinson and J.S. Puttock, "Vented confined explosions involving methane/hydrogen mixtures," *International Journal of Hydrogen Energy,* vol. 36, no. 3, pp. 2337-2343, 2011.

[17] H2 Tools, "Hydrogen Leak Auxillary Building," 2017. [Online]. Available: https://h2tools.org/lessons/hydrogen-leak-auxiliary-building.

[18] H2 Tools, "Leak LHY tank fueling station," 2017. [Online]. Available: https://h2tools.org/lessons/leak-lhy-tank-fueling-station.

[19] H2 Tools, "Hydrogen leakage ground package flow control valve," 2017. [Online]. Available: https://h2tools.org/lessons/hydrogen-leakage-ground-packing-flow-control-valve.

[20] H2 Tools, "Hydrogen Fire valve packing during maintenance shutdown chemical manufacturing plant," 2017. [Online]. Available: https://h2tools.org/lessons/hydrogen-fire-valve-packing-during-maintenance-shutdown-chemical-manufacturing-plant.

[21] J. M. Lawrence and P. G. Fernandes, "A typology of North Sea oil and gas platforms," 2022.

[22] National Grid, "Hydrogen Focus Area," 2022. [Online]. Available: https://www.nationalgrid.com/gas-transmission/future-of-gas/hydrogen.

[23] J. Overton, "Issue Brief | The Growth in Greenhouse Gas Emissions from Commercial Aviation (2019, revised 2022)," EESI: Environmental and Energy Study Institute, 2022. [Online]. Available: https://www.eesi.org/papers/view/fact-sheet-the-growth-in-greenhouse-gas-emissions-from-commercial-aviation.

[24] W. A. Reinsch and W. O'Neil, "Hydrogen: The Key to Decarbonizing the Global Shipping Industry?," [Online]. Available: https://www.csis.org/analysis/hydrogen-key-decarbonizing-global-shipping-industry.

[25] R.K.Gangopadhyaya, S.K.Dasa and M.Mukherjeeb, "Chlorine leakage from bonnet of a valve in a bullet—a case study," *Journal of Loss Prevention in the Process Industries,* vol. 18, no. 4-6, pp. 526-530, 2005.

[26] P. Helsel, "Leaking Valve Suspected in DuPont Chemical Leak That Killed Four," NBC News, 2014. [Online]. Available: https://www.nbcnews.com/news/us-news/leaking-valve-suspected-dupont-chemical-leak-killed-four-n249396.

[27] United States Environmental Protection Agency, "Understanding Global Warming Potentials," 2022.

[28] World Nuclear Association, “World Energy Needs and Nuclear Power,” World Nuclear Association, November 2021. [Online].

[29] International Energy Agency, “Net Zero by 2050 - A roadmap for the Global Energy Sector,” IEA Publications, 2021.

[30] R. G. Derwent, “Hydrogen for heating: atmospheric impacts,” The Department of Business Energy and Industrial Strategy, London, 2018.

[31] GDN Joint Report , “Shrinkage and Leakage Model Review 2018,” 2018.

[32] I. B. Ocko and S. P. Hamburg, “Climate consequences of hydrogen leakage,” *Atmospheric Chemistry and Physics,* 2022.