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Spatially Resolved Optimization for Studying the Role of Hydrogen for Heat Decarbonization Pathways

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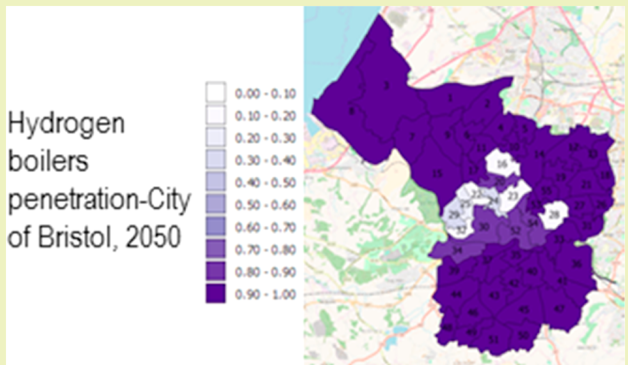
Supporting Information

ABSTRACT: This paper studies the economic feasibility of installing hydrogen networks for decarbonizing heat in urban areas. The study uses the Heat Infrastructure and Technology (HIT) spatially resolved optimization model to trade-off energy supply, infrastructure, and end-use technology costs for the most important heat-related energy vectors: gas, heat, electricity, and hydrogen. Two model formulations are applied to a UK urban area: one with an independent hydrogen network and one that allows for retrofitting the gas network into hydrogen. Results show that for average hydrogen price projections, cost-effective pathways for heat decarbonization toward 2050 include heat networks supplied by a combination of district-level heat pumps and gas boilers in the domestic and commercial sectors and hydrogen boilers in the domestic sector. For a low hydrogen price scenario, when retrofitting the gas network into hydrogen, a cost-effective pathway is replacing gas by hydrogen boilers in the commercial sector and a mixture of hydrogen boilers and heat networks supplied by district-level heat pumps, gas, and hydrogen boilers for the domestic sector. Compared to the first modeled year, CO_2 emission reductions of 88% are achieved by 2050. These results build on previous research on the role of hydrogen in cost-effective heat decarbonization pathways.



KEYWORDS: *Hydrogen, Energy systems model, Heat decarbonization, Networks, Gas, Infrastructure, Spatially resolved*

INTRODUCTION

In the United Kingdom, around 40% of the total energy demand in 2016 was used for heating and hot water in buildings,[1] accounting for approximately 20% of its greenhouse gas emissions.[2] This demand was mainly supplied via natural gas distribution infrastructure and combustion in boilers.[1] According to the Committee on Climate Change,[2] the role of hydrogen for heating and hot water in buildings should be considered in the context of heat decarbonization. Specifically, the decision on converting the existing gas network infrastructure to supply hydrogen in buildings has gained great attention in the year prior to the time of writing.[3]

Several authors are studying scenarios for a technically and economically feasible decarbonization of gas networks through conversion to enable them to transport hydrogen. Dodds and Demoullin[3] assess the technical feasibility of converting the UK gas network to deliver hydrogen for heat by using interviews supported by literature review and then assessing the economic benefit of this option using the UK MARKAL energy system model. They conclude that hydrogen can be distributed safely in low pressure polyethylene pipes and that depending on conversion and capital costs hydrogen micro-combined heat and power (CHP) fuel cells could be a cost-effective heat decarbonization measure. Dodds et al.[4] examine the potential of hydrogen and fuel cell technologies to deliver secure, affordable, and low carbon heat in high-income countries. They argue that hydrogen-fueled fuel cell CHPs have lower net emissions than natural gas-fueled and electricity-based heating systems when considering current electricity generation mixes in most countries. Additionally, they identify a gap in heat decarbonization scenarios produced by energy systems models since fuel cells and hydrogen technologies are not incorporated into the heat supply technology pool and are thus *a priori* disregarded as feasible alternatives.

The H21 Leeds City Gate project[5] studies the technical and economic possibility of converting the existing gas network in Leeds to 100% hydrogen. The UK has been undertaking the Mains Replacement Programme which aims to upgrade most iron distribution pipelines to polyethylene. The study concludes that the new polyethylene gas network has appropriate characteristics for conversion to hydrogen, with minimum reinforcement in certain zones. Likewise, Speirs et

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al.[6] suggest that gas network decarbonization options can be attractive for countries such as the UK that have a well-developed gas network. Additionally, they suggest that even for countries with low gas network penetration the cost of building low pressure hydrogen networks may be competitive compared to other decarbonization alternatives such as installing air-source or ground-source heat pumps.

One of the main concerns of using hydrogen as an energy vector is the issue of safety. According to Dodds and Demoullin,[3] low pressure distribution iron and steel pipes are not safe for transporting hydrogen due to potential embrittlement, although polyethylene pipes do not present this problem. A potential hazard in polyethylene pipes is leakage in connection pipes. According to the H21 Leeds City Gate project,[5] natural gas polyethylene pipe systems can be assessed and retrofitted so that pressures fall within safety limits and leakages in connection pipes are minimized at relatively low average costs per kilometer. They identify however several hydrogen potential safety issues due to its high flammability. Because of this, a hydrogen steam methane reformer or storage locations could present a safety hazard or its potential leakage in domestic properties. However, the HyHouse study conducted by Kiwa Gastec[7] concluded that in spite of its high flammability, as hydrogen has a high stoichiometric mixture together with a low density and high diffusivity, the high concentrations of hydrogen in air required for combustion are very difficultly reached in domestic properties. The H21 Leeds City Gate report claims that this hazard is comparable to other flammable gases such as natural gas and that current natural gas codes in the UK would need to be revised and adjusted for the inclusion of hydrogen. For example, as highlighted by Dodds and Demoullin,[3] as hydrogen is odorless and its flame is invisible, they suggest that hydrogen sensors should be fitted into dwellings and that flame detection should be an issue to further investigate.

At the time of writing, few studies assess hydrogen as an energy vector by considering the whole heat energy system in an integrated and spatially resolved manner. Dodds and McDowall[8] use the UK MARKAL model to study different decarbonization options for the UK gas network, including biomethane, hydrogen injection into natural gas, and converting the gas network into hydrogen. They conclude that converting the gas network to hydrogen is the only possible cost-effective alternative for decarbonizing gas for heating. This research systematically compares different alternatives for heat supply by considering the whole energy system. However, network infrastructures are modeled as energy exchange processes and thus fail to provide spatially explicit solutions. Balta-Ozkan and Baldwin[9] present a framework in which a spatially explicit hydrogen module is included into the UK MARKAL energy system model and explore the trade-offs between production, delivery, and end-use of hydrogen. They characterize the UK hydrogen network with 6 supply and 12 demand centers. However, this coarse spatial resolution does not allow for the evaluation of infrastructure trade-offs at an urban scale and for the assessment of low pressure gas network retrofitting. Moreno-Benito et al.[10] present a spatially explicit multiperiod optimization model to develop a hydrogen supply chain infrastructure and apply this model for analyzing the UK's development of hydrogen infrastructure to obtain a cost-effective transition toward a sustainable hydrogen economy. This research considers regional and local transmission and distribution of hydrogen. However, since it is implemented to evaluate the hydrogen supply chain infrastructure, it does not take into account the other energy vector infrastructures.

This article aims to fill the gap of assessing the cost effectiveness of hydrogen as an energy vector compared with others by considering the whole urban level heat supply system in an integrated manner. The objective is to study the economic feasibility of installing hydrogen networks or retrofitting the existing gas network to transport hydrogen when considering trade-offs in the whole heat supply energy system in a spatially resolved urban area. The study takes into account the trade-offs between district-level and individual-level heat supply technologies and different network infrastructures for a case study in the UK. Two formulations for hydrogen networks are studied in this research: The first formulation allows for installing a hydrogen network that is independent of the gas network. The second formulation allows for retrofitting the existing gas network to carry hydrogen. For both formulations, three scenarios for hydrogen prices and two scenarios for hydrogen equivalent carbon emissions are modeled to determine its influence on cost-effective deployment of hydrogen networks.

The study is structured as follows: The methodology describes briefly the base model used in this research and details the modifications made for the cases of installing or retrofitting hydrogen networks, as well as describing the cases and scenarios studied and input data used. The Results and Discussion section then describes the main results for each case and concludes with insights on the economic feasibility of installing or retrofitting hydrogen networks in the UK.

■ METHODOLOGY

This research modifies the base HIT model presented in ref 11 to include hydrogen networks. The HIT model is a mixed integer linear program that minimizes the total system cost for investment and operation of heat and electricity supply technologies and infrastructure from 2015 through 2050. A region is spatially disaggregated into zones, and topology of the region and zones is characterized in input data. Inputs include heat and electricity demands per zone; gas, heat, and electricity network infrastructure costs; heat supply technology techno-economic parameters; and fuel, electricity, and carbon prices. The model makes investment decisions regarding heat end-use technologies, network infrastructure, and source of energy supply in each 5-year period. It also determines operational decisions for the installed technologies in diurnal and seasonal time slices. Outputs include size and locations of individual and district-level heat supply technologies in each time period, operation of heat supply technologies in each time slice, electricity consumption/generation from/into the grid in each zone and time slice, and carbon emissions. For a full description of the model, the reader is referred to ref 11. The model formulation is included in the Supporting Information.

■ MODIFICATIONS TO THE HIT MODEL

The formulation of the HIT model is detailed in ref 11 which includes gas, electricity, and heat infrastructure. This research modifies the model to include hydrogen networks and hydrogen-fueled heat supply technologies. Two formulations are presented: Formulation A introduces the possibility of including a hydrogen network which is independent from the gas network. Formulation B introduces the possibility of

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including a hydrogen network by retrofitting the existing gas network to convert it into hydrogen (considering that existing low pressure polyethylene gas networks can be converted into hydrogen at relatively low cost compared to the total system cost[5,12]). This section explains the modifications and additions made to the model for this work. The nomenclature used for the model formulation is shown in the Supporting Information.

First, a constraint on operation of individual heat supply technologies following heat load was added. This constraint (eq 1) ensures that each dwelling has an individual heat supply technology. For the gas and hydrogen micro-CHP units, this equation was set as an equality constraint, so that the micro-CHPs are not allowed to dump heat in order to sell electricity. In this equation, $OCHI_{b\ peak\ i_{ind}jy}$ represents the operating capacity of individual heat supply technology i_{ind} for demand type b in zone j which is operating in the peak demand time slice in year y.

$$HP_h \times OCHI_{b\,peak i_{ind}jy} \leq OCHI_{bhi_{ind}jy} \quad \forall\ bhi_{ind}jy \tag{1}$$

The HIT model represents distribution networks in two different ways. Networks within zones are modeled by assuming an average cost per unit length. To estimate the network length that is built within zones, the total road length of the zone is multiplied by the fraction of dwellings that are connected to the given network. This fraction can be estimated as the total installed capacity of technologies connected to the given network over the peak heat demand. For example, if 40% of peak heat demand in a zone is served by heat exchangers and 60% by gas boilers, the length of the heat network and gas network would be 40% and 60% of the zone's total road length, respectively. This length multiplies the average cost per unit length in the cost function. Equation 2 shows the constraint added for the hydrogen network length within each zone. Networks between zones can connect neighbor zone centers. The distance is fixed, and the decision variable for this network element is the network capacity (which eventually translates into pipe or cable diameters). An extra set of network variables representing hydrogen networks was added, together with individual and district-level hydrogen-fueled heat supply technologies. Equation 3 establishes that the network capacity should allow for the energy flow of each energy carrier (gas, electricity, hydrogen, heat) between zones.

$$\frac{\sum_{b,i_{ind}=\text{hyd boilers, hyd micro-CHPs}} TCHI_{bi_{ind}jy}}{\sum_b Dem^H_{b\,peak\ jy} \cdot Num_{bjy}} \times Rl_j = TLN_{j\,hydn\,y} \quad \forall\ jy \tag{2}$$

$$F_{hjj'ny} \leq TCN_{jj'ny} \quad \forall\ hjj'ny \tag{3}$$

For each zone, energy balances for all four energy carriers are performed. The energy balance states that the net energy flow into a zone minus the net energy flow out of a zone must equate the energy consumed from the given network minus the energy injected into the network in the zone. Equation 4 shows the consumed energy in each zone for the hydrogen network. Equation 5 imposes no hydrogen injection into the network based on the assumption that hydrogen is injected via the transmission network from outside the city boundary into the city's hydrogen distribution network.

$$F^{CONS}_{hj\,hydn\,y} = \sum_{b,i_{ind}=\text{hyd boiler, hyd micro-CHP}} \frac{OCHI_{bhi_{ind}jy}}{\eta^{ThI}_{i_{ind}}} + \sum_{T,i_{dist}=\text{hyd boiler dist}} \frac{OCHD_{hi_{dist}jTy}}{\eta^{ThD}_{i_{dist}T}} \quad \forall\ hjy \tag{4}$$

$$F^{GEN}_{hj\,hydn\,y} = 0 \tag{5}$$

Finally, hydrogen-fueled micro-CHPs were added to the equation for electricity generated and injected into the grid in each zone. This is shown in eq 6.

$$F^{GEN}_{hj\,elecn\,y} = \sum_e OCE_{hejy} + \sum_T OCHD_{h\,CHP_{dist}\,jTy} \times \frac{\eta^{ED}_{CHP_{dist}T}}{\eta^{ThD}_{CHP_{dist}T}} + \sum_b OCHI_{bh\,CHP_{indgas}\,jy} \times \frac{\eta^{EI}_{CHP_{indgas}}}{\eta^{ThI}_{CHP_{indgas}}} + \sum_b OCHI_{bh\,CHP_{indhyd}\,jy} \times \frac{\eta^{EI}_{CHP_{indhyd}}}{\eta^{ThI}_{CHP_{indhyd}}} \quad \forall\ hjy \tag{6}$$

Equations 1 to 6 are the additions to the base HIT model for Formulations A and B. The following equations are the supplementary equations introduced for Formulation B, when gas networks can be retrofitted into hydrogen networks. For Formulation B, a proxy network which is the total low pressure network for gas and hydrogen, *HGn*, is introduced as a new element in the network sets. Here, *gasn* and *hydn* continue to represent the net gas and hydrogen networks that fuel heat supply technologies. The *HGn* network represents the total gas network installed, including what is initially gas and then retrofitted into hydrogen. Also, *hydn* is the part of the total low pressure network, *HGn*, that is retrofitted into hydrogen and is represented as an added-on cost; *gasn* is the part of the total low pressure network, *HGn*, that remains as gas network exclusively. Flow balances are performed over heat networks, electricity networks, *gasn*, and *hydn*. All equations that define new installed network lengths and capacities, remaining network lengths and capacities, and decommissioned network lengths and capacities are used to define *gasn* and *hydn* as in Formulation A. The total network capacities and lengths for *HGn* are defined as the sum of the gas and hydrogen network capacities and lengths, as shown in eqs 7 and 8.

$$TCN_{jj'\,HGn\,y} = TCN_{jj'\,gasn\,y} + TCN_{jj'\,hydn\,y} \quad \forall\ jj'y \tag{7}$$

$$TLN_{j\,HGn\,y} = TLN_{j\,gasn\,y} + TLN_{j\,hydn\,y} \quad \forall\ jj'y \tag{8}$$

Finally, the network capital costs are added over the total low pressure network, *HGn*, and over the hydrogen network, *hydn*. The capital cost associated with *HGn* is the average cost for a low pressure polyethylene gas network. The capital cost associated with *hydn* is the average retrofitting cost to convert a gas network into a hydrogen network obtained from ref 6 and shown in Table S6. This cost is the average cost per length that the H21 Leeds City Gate project incurred in, in order to retrofit the natural gas polyethylene pipes to carry hydrogen, by reinforcing connection pipes and critical pressure pipes to ensure safe hydrogen transport. This cost also includes the additional infrastructure needed for medium and low pressure gas networks to be able to supply the necessary hydrogen volumes. Equations for the capital costs and salvage values of

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network infrastructures are shown in eqs 9 and 10. In this way, the proxy network is used to keep track of the real costs and infrastructure lifetimes, while the net gas and hydrogen networks (*gasn* and *hydn*) are used to reflect the net network capacities for energy balances.

$$NTW = \sum_{jj'yn \neq gasn} \frac{ICN_{jj'ny}}{2} \times d_{jj'} \times \mathrm{Cost}_{ny}^{NT} \times \frac{1}{(1+r)^{y}} + \sum_{jyn \neq gasn} NLN_{jny} \times \mathrm{Cost}_{ny}^{ND} \times \frac{1}{(1+r)^{y}} \quad (9)$$

$$\begin{aligned} SLV = {} & \sum_{bi_{ind}jy} VCHI_{bi_{ind}jyy_{final}} \times \mathrm{Cost}_{bi_{ind}jy}^{CI} \times \frac{Lt_{i_{ind}}^{I} - (y_{final} - y)}{Lt_{i_{ind}}^{I}} \\ & \times \frac{1}{(1+r)^{y_{final}}} + \sum_{i_{dist}jTy} VCHD_{i_{dist}jTyy_{final}} \times \mathrm{Cost}_{i_{dist}jTy}^{CD} \\ & \times \frac{Lt_{i_{dist}T}^{D} - (y_{final} - y)}{Lt_{i_{dist}T}^{D}} \times \frac{1}{(1+r)^{y_{final}}} \\ & + \sum_{ejy} VCE_{ejyy_{final}} \times \mathrm{Cost}_{ejy}^{CE} \times \frac{Lt_{e}^{E} - (y_{final} - y)}{Lt_{e}^{E}} \\ & \times \frac{1}{(1+r)^{y_{final}}} + \sum_{jj'yn \neq gasn} \frac{CCN_{jj'nyy_{final}}}{2} \times d_{jj'} \times \mathrm{Cost}_{ny}^{NT} \\ & \times \frac{Lt_{n}^{N} - (y_{final} - y)}{Lt_{n}^{N}} \times \frac{1}{(1+r)^{y_{final}}} \\ & + \sum_{jyn \neq gasn} VLN_{jnyy_{final}} \times \mathrm{Cost}_{ny}^{ND} \times \frac{Lt_{n}^{N} - (y_{final} - y)}{Lt_{n}^{N}} \\ & \times \frac{1}{(1+r)^{y_{final}}} \end{aligned} \quad (10)$$

INPUT DATA AND CASE DESCRIPTION

Formulations A and B were both run for a case study of the City of Bristol. The city was subdivided into its 55 middle layer super output areas (MSOAs).[13] Commercial and domestic gas and electricity annual demand were obtained for each MSOA from refs 14 and 15 and allocated into 16 time slices. Gas demand was converted into heat service demand assuming an efficiency of 81%.[16] Time slices for heat demand allocation were drawn from the UK TIMES model.[17] Electricity demand allocation was obtained from Elexon profile classes[18] which are the profiles used by the electric system operator in the UK to allocate unmetered electricity consumption into profiles.

Table S5 shows the input techno-economic parameters used for heat and electricity supply alternatives. Costs were obtained from different sources and cross-checked with UK TIMES.[17] Constraints were imposed so that only domestic technologies could supply domestic demand and so that only commercial technologies could supply commercial demands. For domestic technologies, unit sizes shown in Table S5 were assumed to serve individual dwellings. Based on the capital cost of technologies for these sizes, domestic costs per peak kW per dwelling were calculated for each zone. For the commercial sector, the capital costs per kW shown in Table S5 were used. Table S6 shows the techno-economic parameters for network infrastructure, and Table S7 shows the prices and emission factors for gas and electricity, together with carbon prices used.

As for gas and electricity, the assumption of the HIT model is that hydrogen is centrally produced and readily available from the transmission system to purchase at retail prices. According to ref 6, as hydrogen production routes vary, retail prices and associated equivalent carbon emissions can vary as well. Estimates for retail hydrogen prices range from 4.9 to 18.4 p/kWh, with an average of 9.3 p/kWh. Equivalent carbon emissions associated with producing hydrogen via steam methane reformers with carbon capture and storage (CCS) range from 23 to 150 gCO2eq/kWh. To tackle these uncertainties, three scenarios for hydrogen retail prices and two scenarios for associated carbon emissions were considered for each formulation. Regarding hydrogen price scenarios, scenario HP1 represents average hydrogen prices as projected in ref 6. Scenario HP2 represents sale price estimates excluding point of conversion as projected in ref 5, and scenario HP3 represents low hydrogen price estimates as projected in ref 6. These are shown in Table S8. Projected retail prices include production costs, transmission costs, distribution costs, taxes, and profits. Distribution costs are then discounted as these are included endogenously through distribution network costs. The two scenarios for equivalent carbon emissions assume the production route is via steam methane reforming with CCS. Scenarios HE1 and HE2 for equivalent carbon emissions are shown in Table S8.

The model was first run for a base year (2013) assuming heat demand was supplied exclusively by gas boilers in order to determine the initial network topology for gas and electricity. This simplification was assumed considering specific sectorial data. According to ref 1, 90% of UK domestic dwellings in 2015 had natural gas boilers to serve their heating demands. In the service sector, 72% of heating and hot water demand was served by natural gas in 2016, presumably via its combustion in gas boilers. Also, as heat demand is estimated from gas consumption data assuming a gas boiler efficiency, the initial gas network topology would effectively reflect the demand for gas. For Formulation A, initial networks were then enforced to be decommissioned linearly from 2015 to 2050. For Formulation B, no decommissioning was enforced, making the implicit assumption that as the Mains Replacement Programme is in place, the new gas network represents a sunken cost and should not be considered in the analysis. Additionally, half of the initial gas boilers were imposed to be decommissioned in 2020 and half in 2025. As shown in Table S5, heat supply hydrogen technologies were made available from 2020 or 2025, depending on the technology.

Figure 1 shows the modeled zones and their linear heat density calculated as annual heat demand divided by the total road length in each zone, obtained from ref 19.

RESULTS AND DISCUSSION

Results for Formulation A when the hydrogen network is independent of the gas network were the same for the three hydrogen price scenarios and for the two hydrogen emission scenarios. For Formulation A, as the gas network is decommissioned toward 2050, gas boilers are replaced by heat exchangers connected to heat networks, together with some commercial air-source heat pumps. No participation of hydrogen technologies is observed in the domestic or commercial sectors. For all these scenarios, heat networks are supplied by air-source heat pumps together with gas boilers, as

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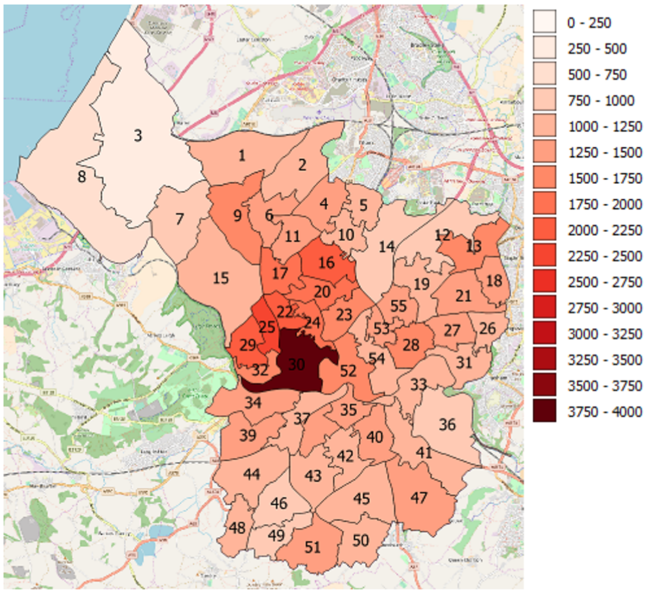

Figure 1. Linear heat density per zone [kWh/m].

shown in Figure 4. Therefore, the lower hydrogen network compared to heat network costs do not offset the lower end-use technology costs (heat exchangers versus hydrogen technologies), together with the gains in efficiency and eventual gains in carbon costs of district-level air-source heat pumps. Additionally, no hydrogen networks are obtained for Formulation B for average hydrogen prices as projected in ref 6 (scenario HP1) when gas networks are allowed to be retrofitted into hydrogen.

Figures 2 and 3 show the total share of individual level heat supply technologies for Formulation B (when gas networks are allowed to be retrofitted into hydrogen networks), for hydrogen emissions scenario HE1, and hydrogen price scenarios HP2 and HP3, respectively. Figure 2 (average hydrogen price scenarios according to ref 5) shows that as gas networks are decommissioned, gas boilers are replaced by heat exchangers connected to heat networks in the commercial and domestic sectors. Additionally, some participation of hydrogen boilers is observed in the domestic sector, reaching 8% of the total heat supply by 2050. Figure 3 shows that for the low hydrogen price case hydrogen boilers completely replace gas boilers in the commercial sector and replace both heat exchangers and gas boilers in the domestic sector, reaching 86% of penetration by 2050. No participation of individual supply gas boilers is observed by 2050, and a lower participation of heat networks is obtained for the domestic sector, compared to the average hydrogen price scenario. For hydrogen price scenario HP2 and low emissions scenario HE2, gas boilers are progressively replaced by a mixture of hydrogen boilers and heat exchangers for both domestic and commercial sectors, reaching hydrogen boiler and heat network uptakes of 38% and 50%, respectively, by 2050.

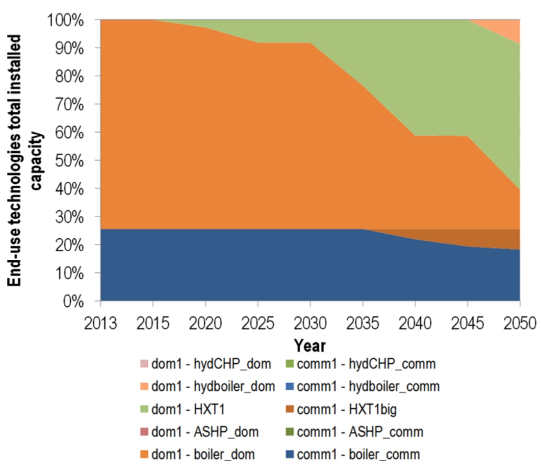

Figure 2. Total share of individual level heat supply technologies. Formulation B: Price scenario HP2 and emission scenario HE1.

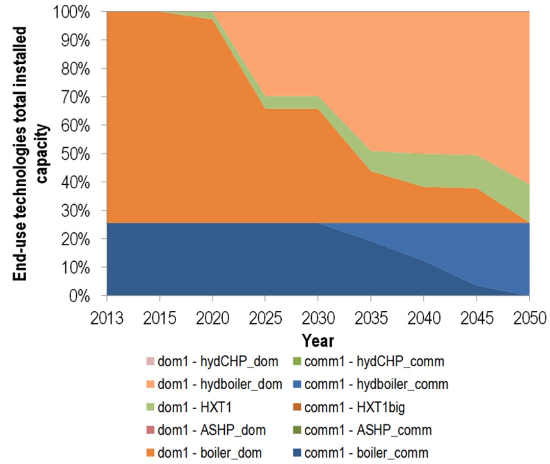

Figure 3. Total share of individual level heat supply technologies. Formulation B: Price scenario HP3 and emission scenario HE1.

Figure 4 shows the total capacity of district-level heat technologies supplying heat networks for Formulation A (all scenarios). Most district heat networks are supplied by a combination of natural gas district boilers and district-level air-source heat pumps. No hydrogen boilers are observed, even though capital costs and efficiency of both hydrogen and natural gas district-level boilers are assumed to be equal. This shows that the lower hydrogen carbon emissions do not offset its higher price compared to natural gas. For Formulation B (hydrogen price scenarios HP1 and HP2 and both emission scenarios), although the capacities differ from those of Figure 4, the same tendency of heat networks being supplied by air-source heat pumps and gas boilers is observed.

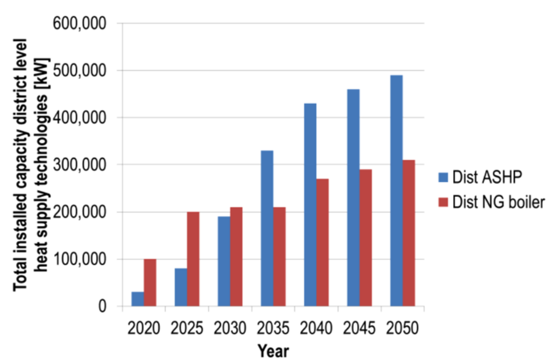

Figure 4. District-level heat supply technologies. Formulation A: All scenarios.

Figure 5 shows the total capacity of district-level heat technologies supplying heat networks for Formulation B (price scenario HP3 and emission scenario HE1). District heat

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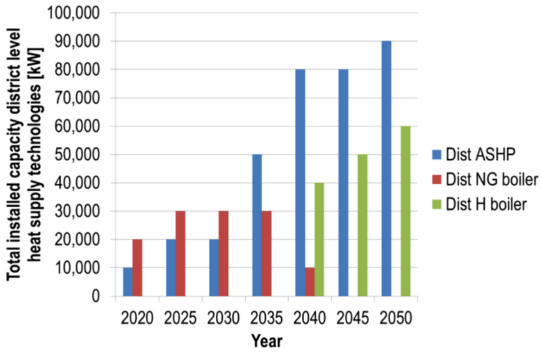

Figure 5. District-level heat supply technologies. Formulation B: Price scenario HP3 and emission scenario HE1.

networks are supplied by a combination of district boilers and district-level air-source heat pumps as for the previous formulations and scenarios. However, this figure shows that for low hydrogen prices not only a high participation of hydrogen boilers at the domestic heat supply level is observed as discussed previously but also at the district-level hydrogen boilers replace gas boilers for supplying heat networks.

Figure 6 shows the heat network penetration per zone by 2050 for Formulation A (all scenarios). Comparing this figure

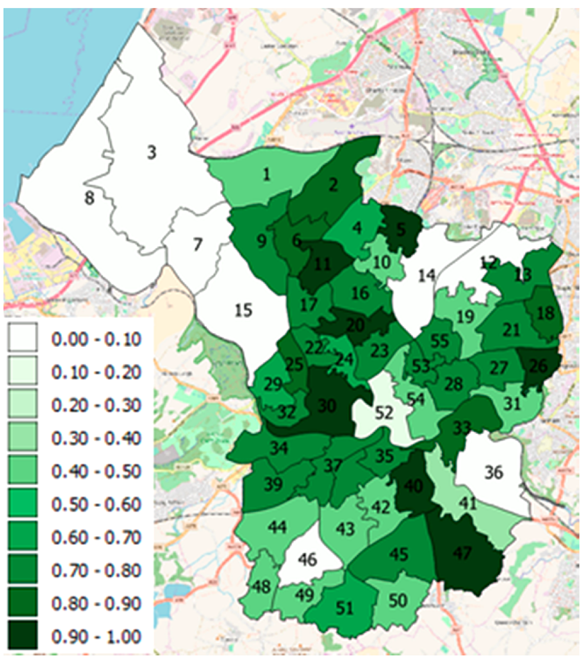

Figure 6. Heat network penetration, 2050. Formulation A: All scenarios.

with Figure 1, it is observed that there is a strong correlation between heat network penetration and linear heat density. For these scenarios of techno-economic parameters, heat network penetrations over 60% are cost effective by 2050 in zones with linear heat densities higher than 1250 kWh/m, while linear heat densities over 2250 kWh/m imply a cost-effective heat network penetration of over 80%. The correlation between heat network penetration and linear heat network arises from the fact that while individual dwelling heat exchange interface units and meters are relatively cheap compared to other individual-level technologies, the associated network infrastructure is high compared to the other alternatives. Thus, high linear heat densities are required to offset high heat network infrastructure costs. For these cases, no hydrogen networks were observed to be cost effective.

Figures 7 and 8 show the heat network penetration and hydrogen boiler penetration per zone by 2050 for Formulation

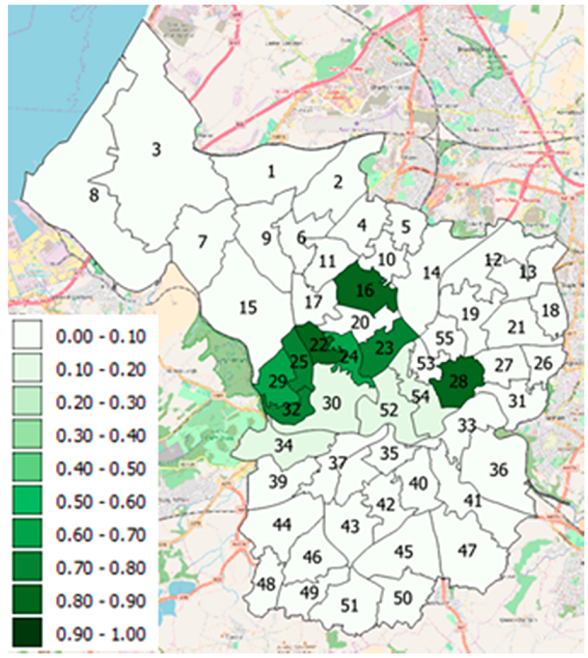

Figure 7. Heat network penetration, 2050. Formulation B: Price scenario HP3 and emission scenario HE1.

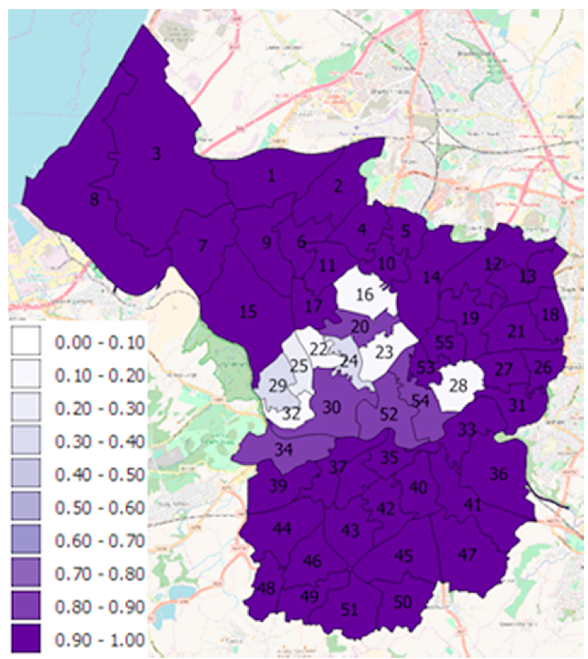

Figure 8. Domestic hydrogen boiler penetration, 2050. Formulation B: Price scenario HP3 and emission scenario HE1.

B (hydrogen price scenario HP3 and emissions scenario HE1). For this low hydrogen price scenario, a high hydrogen boiler penetration was observed throughout zones when the gas network was allowed to be retrofitted into hydrogen. As analyzed before, all zones adopt either heat networks or

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hydrogen boilers, displacing natural gas completely by 2050. This heat supply mix achieves a reduction of 8% in equivalent carbon emissions compared to the average hydrogen price scenario and an 88% reduction by 2050 compared to the first modeled year, 2013. For this case, a high heat network uptake of between 60% and 90% is observed to be cost effective in a relatively intermediate to high linear heat density range from 2000 to 2500 kWh/m.

Finally, it is important to highlight that all the results presented here are sensitive to input techno-economic parameters for technology and network infrastructure costs and to demand topology. Therefore, the results presented are specific for the input parameters used in this research. With these assumed inputs, it is concluded that cost-effective decarbonization pathway is achieved by a mixture of energy carriers and heat supply technologies. For high average hydrogen price estimates, a cost-effective pathway for heat decarbonization toward 2050 is replacing gas boilers by air-source heat pumps and heat networks supplied by a combination of district-level heat pumps and gas boilers. No participation of hydrogen networks is observed when hydrogen is built as an independent network. However, at lower estimates of average hydrogen prices or low hydrogen price scenarios, the gas network is incrementally replaced by hydrogen boilers and heat networks when the gas network is allowed to be retrofitted into hydrogen. Also, an uptake of district-level hydrogen boilers supplying heat networks is observed for low hydrogen prices to the detriment of gas boilers, obtaining a heat network heat supply of mainly district-level air-source heat pumps and hydrogen boilers. This shows that retrofitting the existing gas network into hydrogen is a cost-effective heat decarbonization pathway for the UK, when hydrogen retail prices are in the average to low range. These results are consistent with those from Dodds and McDowall,[8] Speirs et al.,[6] or Sadler et al.,[5] who conclude that there is an opportunity to re-evaluate the Iron Mains Replacement Programme in order prepare the gas infrastructure for a more sustainable hydrogen network. Future work includes introducing future demand for hydrogen fuel cell vehicles in order to explore potential synergies between fuel charging and heat infrastructure for hydrogen. As concluded by Dodds and Ekins,[20] introduction of fuel cell vehicles should be internalized in energy systems models, as an early adoption would enable optimum penetration. Another extension of this work is modeling transmission and hydrogen production facilities, including location constraints that guarantee safe hydrogen production and storage facilities.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acssuschemeng.7b03970.

Nomenclature: Table S1, sets; Table S2, decision variables; Table S3, scalars; and Table S4, parameters. Optimization model formulation. Techno-economic parameters used for modeling: Table S5, heat and electricity end-use and district-level technology techno-economic parameters; Table S6, network parameters; Table S7, gas, electricity, and carbon techno- economic parameters; and Table S8, hydrogen price and emission scenarios. (PDF)

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Notes

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■ REFERENCES

(1) Department for Business EIS. Energy Consumption in the UK (ECUK) 2017 Data Tables. https://www.gov.uk/government/statistics/energy-consumption-in-the-uk (accessed April 2018).

(2) Committee on Climate Change. *Next Steps for UK Heat Policy*, 2016.

(3) Dodds, P. E.; Demoullin, S. Conversion of the UK gas system to transport hydrogen. *Int. J. Hydrogen Energy* **2013**, *38* (18), 7189−7200.

(4) Dodds, P. E.; Staffell, I.; Hawkes, A. D.; Li, F.; Grünewald, P.; McDowall, W.; et al. Hydrogen and fuel cell technologies for heating: A review. *Int. J. Hydrogen Energy* **2015**, *40* (5), 2065−2083.

(5) Sadler, D.; Cargill, A.; Crowther, M.; Rennie, A.; Watt, J.; Burton, S., et al. *H21 Leeds City Gate Northern Gas Networks*, 2016.

(6) Speirs, J.; Balcombe, P.; Johnson, E.; Martin, J.; Brandon, N.; Hawkes, A. *A Greener Gas Grid: What Are the Options? White Paper*; Sustainable Gas Institute, Imperial College London, 2017.

(7) Crowther, M, Orr, G.; Thomas, J.; Stephens, G.; Summerfield, I. *Energy Storage Component Research & Feasibility Study Scheme HyHouse Safety Issues Surrounding Hydrogen as an Energy Storage Vector*; Kiwa Gastec, 2015.

(8) Dodds, P. E.; McDowall, W. The future of the UK gas network. *Energy Policy* **2013**, *60*, 305−316.

(9) Balta-Ozkan, N.; Baldwin, E. Spatial development of hydrogen economy in a low-carbon UK energy system. *Int. J. Hydrogen Energy* **2013**, *38* (3), 1209−1224.

(10) Moreno-Benito, M.; Agnolucci, P.; Papageorgiou, L. G. Towards a sustainable hydrogen economy: Optimisation-based framework for hydrogen infrastructure development. *Comput. Chem. Eng.* **2017**, *102*, 110−127.

(11) Jalil-Vega, F.; Hawkes, A. D. Spatially resolved model for studying decarbonization pathways for heat supply and infrastructure trade-offs. *Appl. Energy* **2018**, *210*, 1051−1072.

(12) Alternatives EEC. *Heat Pumps in District Heating*; 15D/537; 2016 .

(13) Office for National Statistics. Super Output Area (SOA). http://www.ons.gov.uk/ons/guide-method/geography/beginner-s-guide/census/super-output-areas--soas-/index.html (accessed 25 May 2015).

(14) Department of Energy & Climate Change. Sub-national gas consumption data 2013, updated 26 March 2015. https://www.gov.uk/government/collections/sub-national-gas-consumption-data (accessed 12 April 2015).

(15) Department of Energy & Climate Change. Sub-national electricity consumption data 2013, updated 26 March 2015. https://www.gov.uk/government/collections/sub-national-electricity-consumption-data (accessed 12 April 2015).

(16) Keirstead, J.; Calderon, C. Capturing spatial effects, technology interactions, and uncertainty in urban energy and carbon models: Retrofitting newcastle as a case-study. *Energy Policy* **2012**, *46* (0), 253−267.

(17) UCL. Development of the UK TIMES energy systems model 2015. https://www.bartlett.ucl.ac.uk/energy/research/themes/energy-systems/uk-times (accessed 26 January 2016).

(18) ELEXON. Elexon-Profiling 2015. https://www.elexon.co.uk/reference/technical-operations/profiling/ (accessed 8 Sepetember 2015).
(19) OS MasterMap ITN Layer, Shape geospatial data. http://digimap.edina.ac.uk/os (accessed May 2017).
(20) Dodds, P. E.; Ekins, P. A portfolio of powertrains for the UK: An energy systems analysis. *Int. J. Hydrogen Energy* **2014**, *39* (26), 13941−13953.

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