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Research Article

Modelling underground coal gasification: What to start with

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Abstract

Underground coal gasification (UCG) is widely regarded as a clean coal technology that holds enormous potential to decarbonize the world's coal industry. It converts coal underground into combustible syngas through a set of complex physiochemical events. Experimental and numerical efforts over the past century have contributed to the development of UCG around the world; however, tapping the world's deep-situated coal resources with UCG requires substantial contributions from numerous high-quality researchers. To facilitate effective engagement, this paper will provide a background on where to start if one wishes to undertake UCG modelling. First, a brief description of the fundamental phenomena involved in UCG is given. Then, a succinct introduction of the widely used modelling software is rendered, followed by a description of UCG studies to provide insight how to tune the various software packages for modelling UCG and where their strengths lie. This paper shall serve as guidance to new UCG modellers.

Keywords: Underground coal gasification; Modelling; Coal decarbonization; Clean coal technology

1. Introduction

1.1. Climate change and coal

The industrialization of the world's economies over the past two centuries has contributed to an appreciable increase in atmospheric CO_2 concentration, from approximately 280 ppm in pre-industrial times to approximately 410 ppm in recent years [1,2]. Fig. 1 presents a world map of cumulative carbon emissions since 1750 [3], which conveys the overarching contributions from the industrialized economies, namely the United States and Europe. Concomitant to increasing atmospheric CO_2 levels is an increase in the average global temperature, presently approximately 1 °C above pre-industrial levels, and without intervention is poised to reach or surpass 2 °C above pre-industrial levels in the second half of this century; this threshold must not be surpassed to limit the adverse consequences of climate change [4].

The world has reached a consensus to take prompt action to counter climate change. The Intergovernmental Panel on Climate Change recently reported that, to keep global warming less than 1.5 °C above pre-industrial levels, by 2030 the global population needs to cut detrimental anthropogenic CO_2 emissions by 45 % from 2010 levels and reach zero emissions around 2050 [5]. Maintaining concentrations of

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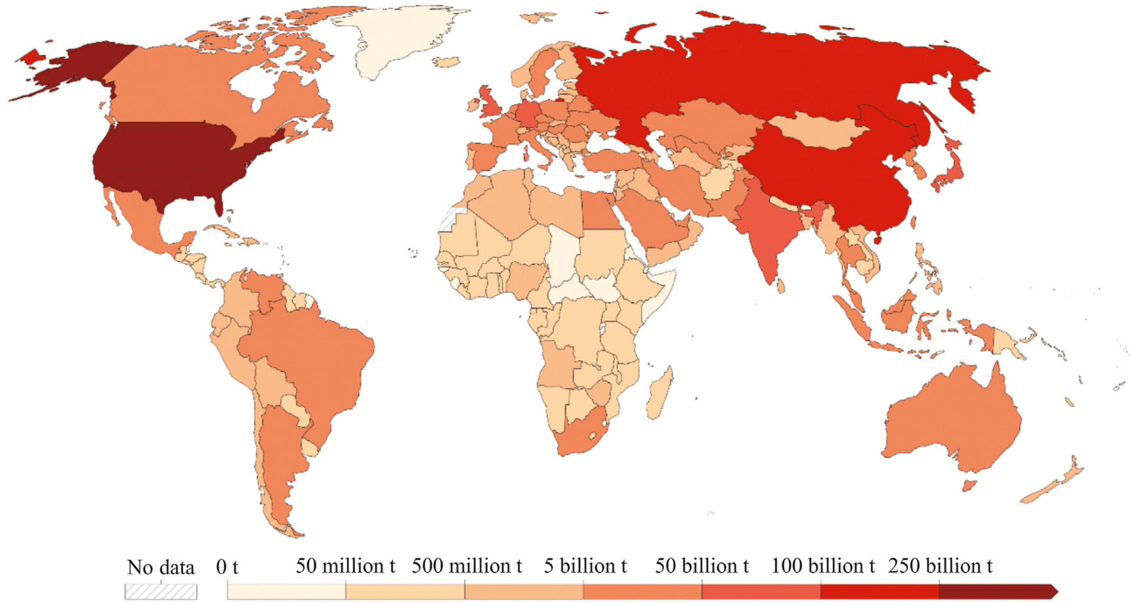

Fig. 1. World map of cumulative CO_2 emissions from 1750 to 2021 [1].

CO_2 in the atmosphere well below 500 ppm throughout the 21st century is pivotal to suppressing the global temperature increase to less than 2 °C above pre-industrial levels [1]. Confounding the efforts for climate change mitigation is the world's heavy reliance on fossil fuels, as illustrated in Fig. 2 [6], which categorically shows that the use of fossil fuels is the main cause of carbon emissions for all states. Emerging powers such as China and India largely depend on coal, whereas developed nations have been successful in coal phase-out. Endowed with rich coal resources, China and India will have to use coal to satisfy their fast-growing economies for the foreseeable future. For example, as shown in Fig. 3 [7], China's use of coal is intertwined in various sectors and industries. Therefore, there is a strong case for the clean use of coal to significantly reduce its carbon footprint; for example, by using underground coal gasification (UCG).

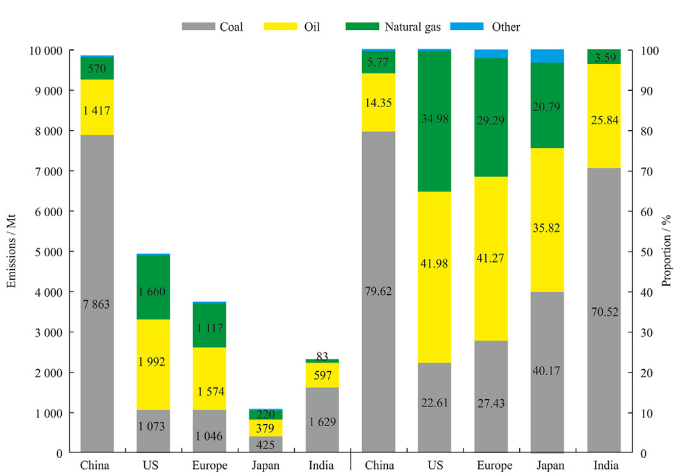

Fig. 2. Carbon emissions of the major nations/regions by fuel in 2019 [6].

1.2. Underground coal gasification and its position

UCG is increasingly recognized as one of the most prospective clean coal technologies for decarbonizing the world's coal industry, with a huge promise to tap coal seams either too deep or uneconomic to mine [8]. It enables the chemical extraction of coal energy in situ without mining [9]. As shown in Fig. 4 [10], coal seams situated deep underground can be recovered using a modern UCG technique, where directional drilling is used to drill an injector and a producer well into

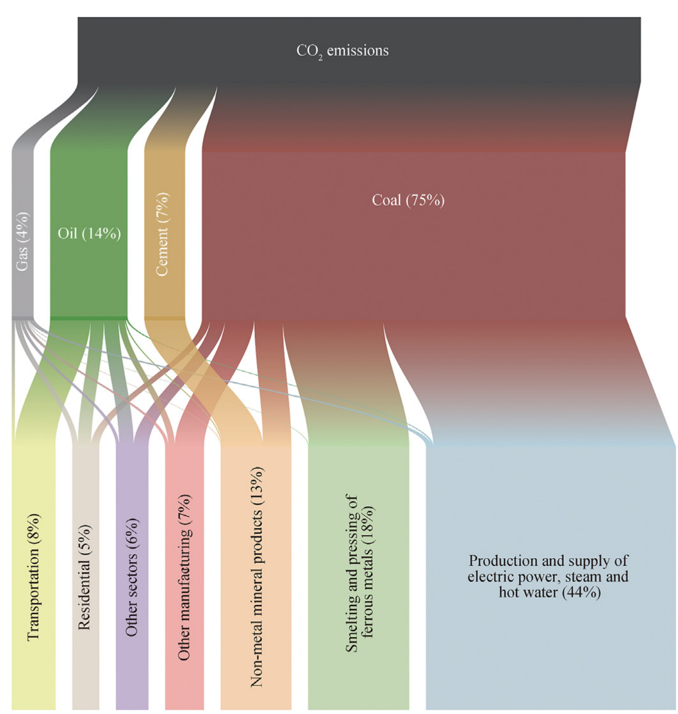

Fig. 3. China's CO_2 emissions flow from sources to sectors in 2017 [7].

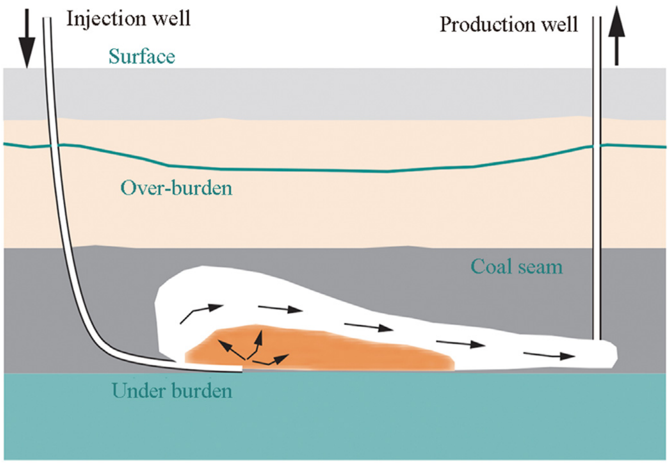

Fig. 4. Schematic of an underground coal gasification process [10].

underground coal seams. Through the injector, the oxidant and steam are brought downhole for the ignition and combustion of coal. Under suitable conditions, a set of chemical reactions occurs to generate a stream of flammable gases (i.e., syngas) comprising hydrogen, methane, carbon monoxide, carbon dioxide, nitrogen, and a trace amount of hydrogen sulfide [11,12]. The relative content of product species is highly dependent on operational parameters, coal properties, and the hydro-geological settings [13].

Since the conceptualization of UCG, numerous field-scale UCG tests have been operated in coal seams around the world. Table 1 lists some of the most important UCG tests [14,15]. Most early work was conducted in the western nations; however, China has recently led the world in the research and development of UCG because of its strong commitment to decarbonizing the use of its vast coal resources [15]. Specifically, China has stressed the strategic importance of UCG as a vital means to decarbonize its use of coal resources in the Five-year Plan (2021–2025) on Energy Technology Innovation and the Energy Technology Innovation Plan of Action (2016–2030).

1.3. Sustainability of UCG

Compared with conventional mining techniques, UCG boasts multifaceted environmental advantages, including health and safety merits, low environmental footprint, the ability to recover of a wide range of resources, process efficiency, and economic potential [11,16,17]. The Lawrence Livermore National Laboratory assessed that recoverable coal reserves in the United States could be increased by 300 % with UCG. In addition, studies have substantiated the use of UCG to enhance hydrogen production [18,19], mobilize heavy oil in a contiguous reservoir [13], and sequester large-scale carbon dioxide securely and permanently [20–27]. A possible pathway to link UCG with carbon dioxide storage and sequestration (CCS) in post-UCG cavities is shown in Fig. 5. An integration of CCS into the UCG system further reduces or eliminates the environmental footprint, therefore making UCG even more advantageous in the market of a carbon-constrained world. A thorough analysis of the sustainability of UCG is provided elsewhere [11].

2. Modelling underground coal gasification: tools in the box

UCG is widely identified as a promising clean coal technology to satisfy the growing energy need of nations while reducing carbon emissions. Nevertheless, it is inherently a very complex process involving a set of coupled physiochemical phenomena. A UCG operation generally proceeds in the subsurface with few operatable factors available. Small-scale laboratory experiments have played a significant role in understanding the multifaceted aspects of UCG, because pilot-scale tests are time-consuming and cost-ineffective. A representative dimension of laboratory-scale experiments is several meters in length and 1–2 m in width and height, as shown in Fig. 6 [28]. The China University of Mining and Technology has a world-class UCG modelling facility in China, and the UCG apparatus at the Central Mining Institute of Poland is reported to be capable of modelling high-pressure, high-temperature conditions [29,30] (see Fig. 7).

Investigation of UCG on a large scale frequently resorts to mathematical methodologies. Early analytical models featured UCG representation in 1D or 2D domains [12]. Later, improvements in computing power and the advent of commercial simulators facilitated the numerical development of UCG in a multidimensional domain. This section provides a background for the reader to start with if they wish to engage in advancing the numerical simulation of UCG. First, a succinct analysis of the fundamental phenomena of UCG is given from a modelling perspective. The popular numerical modelling tools are then briefly introduced, and studies applying each of the simulations are rendered.

2.1. Fundamental phenomena

The overarching physiochemical events in UCG are the pyrolysis of underground coal and the ensuing gasification reactions in a spatial and temporal domain, as illustrated in Fig. 8 [10]. The coal/char reactivity and gasification kinetics govern the rate of chemical reactions. Mass and heat transport are often limiting factors because of the porous structure of coal/char, as well as the presence of a bottom permeable bed made up of falling ash, coal/char rubble, and later, the spalling caprocks. While the gasification of coal/char is a dominant mechanism of cavity growth, research has shown that coal and rock spalling through thermo-mechanical failure is often significant. Within the cavity, drastic chemical reactions take place and transport phenomena are intense. In general, mass flows in the form of convection and diffusion whereas heat transport proceeds through convection, conduction, and radiation. Mass and heat transport are strongly coupled, and thermally induced fractures may play an important role. A detailed description of the fundamental phenomena in UCG can be referred to elsewhere [11,12,17]. Therefore, a good

Table 1
Globally significant underground coal gasification tests [14,15].

Country	Site	Startup year	Coal type	Technique	Injected gas	Seam depth(m)	Seam thickness(m)
Former U.S.S.R.	Lisichansk	1935	Bit.	SDB	Air	30	1
	Podmoskovna	1947	L	LVW	Air	55	3
	Yuzno-Abinskaja	1955	Bit.	SDB	Air	~100	3
	Shatskaya	1959	L	LVW	Air	50	2
	Angrenskaja	1961	L	LVW	Air	150	9
USA	Hanna I	1973	HVC	LVW	Air	120	9
	Hanna II	1975	HVC	LVW	Air	85	9
	Hanna III	1977	HVC	LVW	Air	85	9
	Hoe Creek I	1976	HVC	LVW	Air	40	8
	Hoe Creek IIA	1977	HVC	LVW	Air	40	8
	Hoe Creek IIB	1977	HVC	LVW	O_2/H_2O	40	8
	Hoe Creek IIIA	1979	HVC	LVW	Air	40	8
	Hoe Creek IIIB	1979	HVC	LVW	O_2/H_2O	40	8
	Pricetown I	1979	Bit.	LVW	Air	270	2
	Rawlins IA	1979	SB	SDB	Air	105	18
	Rawlins IB	1979	SB	SDB	O_2/H_2O	105	18
	Centralia A	1984	SBC	K-CRIP	O_2/H_2O	75	6
	Centralia B	1984	SBC	LVW	O_2/H_2O	75	6
	Rocky Mountain IA	1987	SB	K-CRIP	O_2/H_2O	110	7
	Rocky Mountain IB	1987	SB	LVW	O_2/H_2O	110	7
UK	Newman-Spinney P5	1949	SB	BH	Air	75	1
Belgium	Thulin	1986	A	LVW	Air	860	6
Spain	El Tremedal	1997	SB	L-CRIP	O_2/H_2O	580	2
Poland	Wieczorek	2014	SB	SM	Air, O_2, CO_2	464	5.5
China	Xinhe	1994	Bit.	LT	Air/Steam	80	3.5
	Liuzhuang	1996	HVC	LT	Air/Steam	100	3
	Xinwen	2000	HVC	LT	Air/Steam	100	1.8
	Feichang	2001	Bit.	LT	Air	90	1.5
	Xiyang	2001	A	LT	Air/Steam	190	6
Australia	Chinchilla G1	2000	SB	LVW	Air	132	10
	Chinchilla G3	2007	SB	LVW	Air	132	10
	Chinchilla G4	2009	SB	P-CRIP	Air	132	10
	Chinchilla G5	2011	SB	L-CRIP	Air&O_2/H_2O	132	5.5
	Bloodwood Ck, Panel 1	2009	SB	P-CRIP	Air&O_2/H_2O	200	9
	Bloodwood Ck, Panel 2	2011	SB	P-CRIP	Air	200	9
Canada	Swan Hills	2011	HVB	L-CRIP	O_2/H_2O	1400	4.5

Guide to symbols Coal type: L = lignite, SB = subbituminous, SBC = subbituminous C, Bit. = bituminous, HVB = high volatile bituminous B, A = Anthracite. Technique: LVW = linked vertical wells, CRIP = controlled retracting injecting point, L-CRIP = linear CRIP, P-CRIP = parallel CRIP, K-CRIP=Knife-edge CRIP, SDB = steeply dipping beds, BH = borehole method, LT = long tunnel, SM = shaft method.

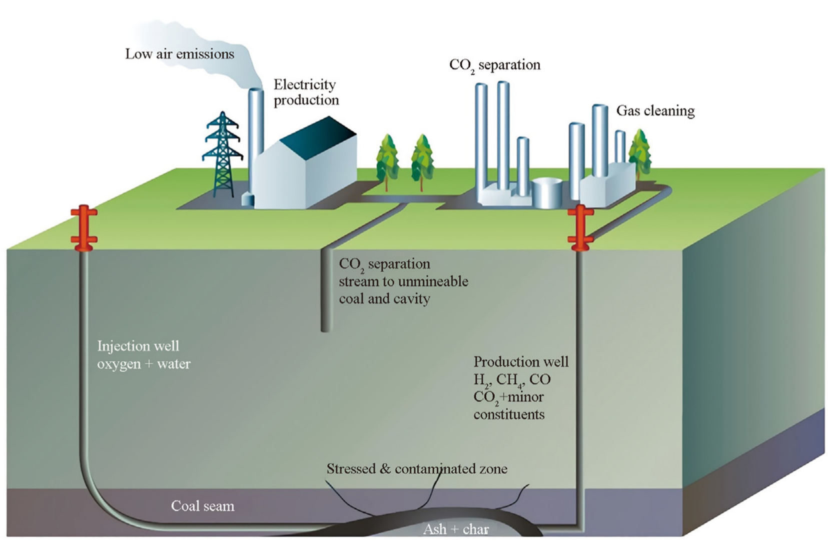

Fig. 5. Conceptualization of linking carbon dioxide storage and sequestration with underground coal gasification (courtesy of the UCG Association).

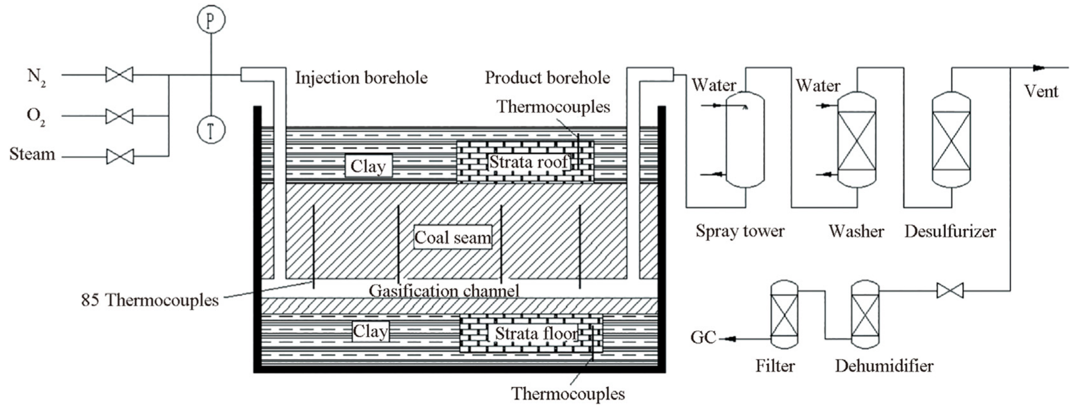

Fig. 6. Representative laboratory-scale underground coal gasification experimental apparatus [28].

modelling tool should be capable of simulating some, if not all, of the underlying phenomena in UCG.

2.2. Tools in the box

Because of the intricate nature of UCG, modellers have used various available tools to examine different aspects of UCG. The popular software packages used with UCG are COMSOL Multiphysics, Ansys Fluent, CMG STARS, FLAC3D, and MODFLOW. Roullier performed a simple analysis of the capabilities and features of some of the tools used for modelling UCG [31], as shown in Table 2. Notably, although not purposefully built for modelling UCG, each modelling tool has its own strengths and weaknesses. This section will help researchers determine suitable modelling tools for the objectives of their respective UCG studies. The organization of the section begins with a brief introduction of the software, followed by some supporting UCG studies from which insights can be gained on how to tune the software for modelling UCG and where its strengths lie. It is beyond the aim of this work to provide a full list of UCG modelling investigations.

2.2.1. COMSOL multiphysics

COMSOL Multiphysics is a comprehensive software package used for finite element analysis, simulation, and solving various physics and engineering problems. It is particularly well-suited for studying coupled phenomena and multiphysics interactions. The software provides intuitive user interfaces based on conventional physics principles and supports the handling of coupled systems of partial differential equations (PDEs). With a unified workflow, it accommodates applications in electrical, mechanical, fluid dynamics, acoustics, and chemical domains. In addition to predefined application modules, the core Multiphysics package enables the solution of PDEs in a weak form, offering flexibility in addressing classical problems. External control of the software is possible through the API for Java and LiveLink for MATLAB, as well as LiveLink products for major CAD software. To develop specialized simulation apps for specific domains, an Application Builder is available, offering drag-and-drop tools (Form Editor) or programming options (Method Editor). For managing COMSOL simulation applications, COMSOL Server is a separate software solution. The software offers various modules, categorized according to different application areas, such as Electrical, Mechanical, Fluid, Acoustic, Chemical, Multipurpose, and Interfacing.

As a potent modelling tool, COMSOL Multiphysics is widely used in essentially all fields of engineering and is one of the most-used packages for UCG applications. Table 3 indicates some studies that use COMSOL Multiphysics. During the past two decades, COMSOL Multiphysics has had good application in modelling UCG. However, most of the models created with COMSOL Multiphysics are 2D, and do not consider chemical reactions. Instead, because COMSOL disallows the solid part of porous media to participate in

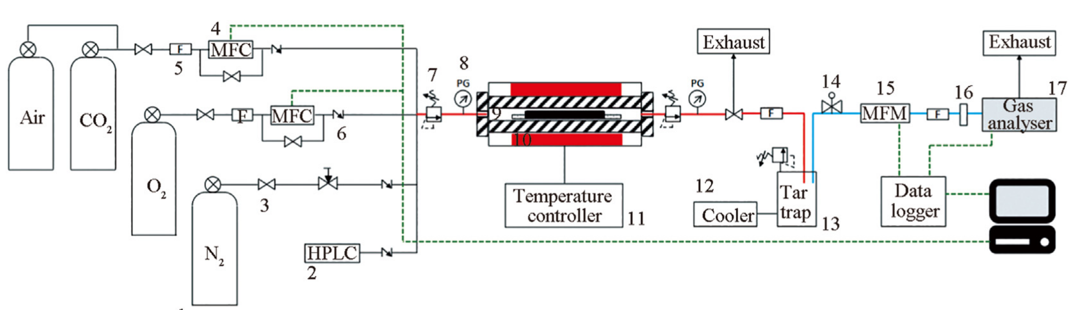

Fig. 7. Ex-situ gasifier for high-pressure high-temperature underground coal gasification in Poland [29,30].

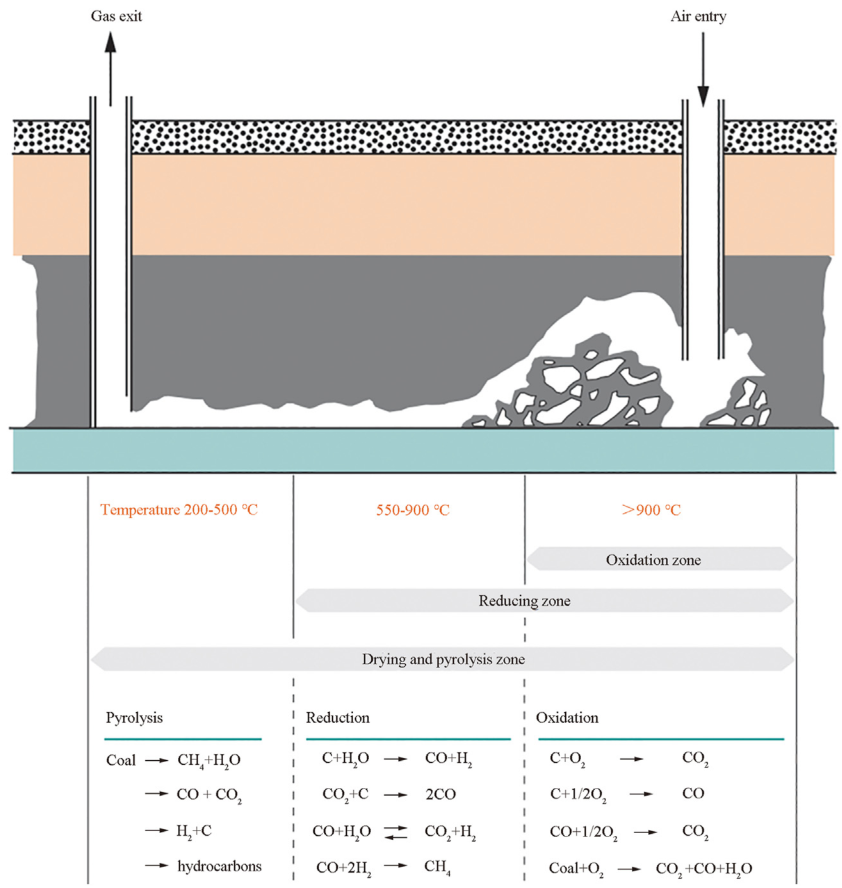

Fig. 8. Schematic of the significant events in underground coal gasification [10].

reactions, modellers resort to a moving heat source to mimic the complex chemical reactions in UCG, which presents an oversimplification of the problem. Some studies have involved coupling COMSOL Multiphysics with another software package such as MATLAB or FLAC3D. In-depth studies of COMSOL Multiphysics–based UCG modelling can be found in graduate dissertations [42–48], most of which are from the China University of Mining and Technology, indicating China's active interest in UCG for decarbonizing its coal industry. Fig. 9 provides a graphical example of modelling UCG with COMSOL Multiphysics based on the study in Ref. [37].

2.2.2. Ansys Fluent

Ansys Fluent is a versatile computational fluid dynamics (CFD) software package designed to simulate and analyze fluid flow, heat and mass transfer, chemical reactions, and other related phenomena. Its comprehensive capabilities include advanced physics modeling, encompassing turbulence modeling, single and multiphase flows, combustion, battery modeling, and fluid–structure interaction. Fluent is distinguished by its modern and user-friendly interface, which optimizes the entire CFD process from pre-to post-processing within a unified workflow presented in a single window. The

Table 2
Comparison of some software packages for modelling underground coal gasification [31].

Software	Method	Dimensions	Cost	Ease of Use	Capabilities			
					Thermal	Hydraulic	Chemical	Mechanical
3DEC	DEM	3D	£18,750	Difficult	Poor	Poor	None	Good
Abaqus	FEM & CFD	3D	Already Owned	Simple	Good	Good	None	Poor
Ansys	FEM & CFD	3D	£500 p.a.	Moderate	Good	Good	None	Poor
COMSOL Multiphysics	FEM & CFD	3D	£6500	Simple	Good	Good	Poor	Poor
FLAC	FDM	2D	£6675	Moderate	Poor	Poor	None	Poor
FLAC3D	FDM	3D	£13,350	Moderate	Poor	Poor	None	Poor
MODFLOW & MT3DMS	FDM	3D	Free	Simple	Good	Good	Good	None
PFC	DEM	3D	Already Owned	Moderate	None	Poor	None	Poor
UDEC	DEM & FDM	2D	Already Owned	Moderate	Poor	Poor	None	Good
In-House	Various	2D, 3D	Free	Very Difficult	Unknown	Unknown	Unknown	Unknown

Table 3
COMSOL Multiphysics−based underground coal gasification studies.

Ref	Year	Objective	Model feature
[32]	2011	to model the transport effects of ash layer	2D, Incompressible laminar flow
[33]	2011	to model cavity growth	2D, moving boundary controlled via MATLAB
[34]	2012	to model heat profile in the overburden rock	2D, heat source instead of chemical reactions
[35]	2012	to model thermal-mechanical damage in the cap rock	2D, thermal-mechanical model via heat coupling with MATLAB (no chemical reactions)
[36]	2014	to model cap rock subsidence	2D, used only heat source function from COMSOL instead of chemical reactions
[37]	2015	to predict the thermo-geomechanical response of the strata	2D, heat source instead of chemical reactions
[38]	2016	to simulate temperature field	2D, heat source instead of chemical reactions
[39]	2017	to simulate temperature field in the caprock	2D, heat source instead of chemical reactions
[40]	2020	to maximize calorific value of syngas	3D, with homogeneous and heterogeneous reactions
[41]	2020	to model thermal-mechanical coupling in strata	2D, heat source instead of chemical reactions
[42]	2021	to predict oxygen flow in the cavity	3D, heat source instead of chemical reactions

software's efficiency is evident in its excellent high-performance computing scaling, allowing for the seamless resolution of large models using multiple processors on both CPUs and GPUs. Users have the flexibility to choose from various solver options, such as pressure-based and density-based CPU solvers, which cater to a wide range of flow scenarios from low-speed to hypersonic flows. Additionally, Fluent offers a native GPU solver based on pressure-based methods, further enhancing computational speed and performance.

Because it is a popular, powerful CFD software, researchers around the world use Ansys Fluent to model the UCG process, with a particular interest in elucidating the complex transport phenomena within the underground cavity, as shown in Table 4. It is also possible to examine UCG in a multidimensional domain with the aid of Ansys Fluent. While both homogeneous and heterogeneous reactions can be included, Ansys Fluent is generally incapable of modelling coal pyrolysis. Therefore, some form of approximation is required to simulate coal consumption for cavity growth prediction. The strength of Ansys Fluent to describe complex flow characteristics in the UCG cavity is presented in Fig. 10 [50].

2.2.3. CMG STARS

Computer Modelling Group Ltd. (CMG) offers the STARS simulator, a powerful reservoir simulation software package with extensive capabilities in modeling thermal and advanced processes. This new generation reservoir simulator is equipped with robust reaction kinetics and geomechanics functionalities. STARS presents various options to cater to complex reservoir scenarios, including chemical and polymer flooding, thermal applications, steam injection, horizontal wells, dual porosity/permeability, directional permeabilities, flexible grids, and fireflood. Its versatility allows for the simulation of diverse processes, such as steam flood, steam cycling, steam with additives, dry and wet combustion, and various chemical

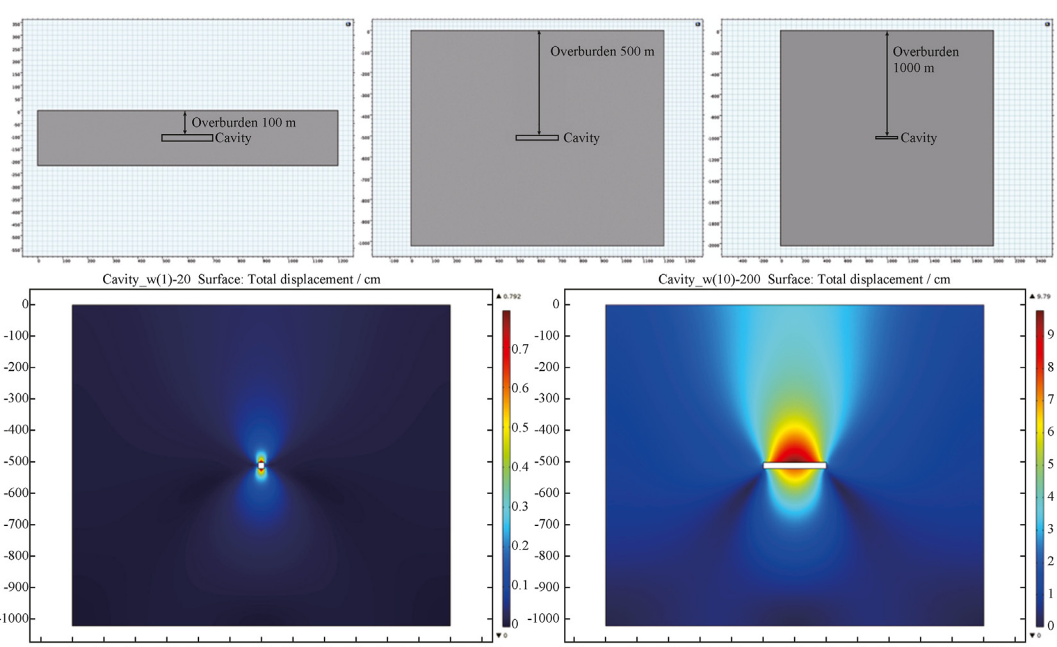

Fig. 9. An example of underground coal gasification modelling with COMSOL Multiphysics [37].

Table 4
Underground coal gasification models using Ansys Fluent.

Ref	Year	Objective	Model feature
[49]	2011	to model reactant gas flow characteristics in cavity	3D, compartment model, isothermal cavity, no chemical reactions
[50]	2012	to model reactant gas flow characteristics in cavity	3D, compartment model, no chemical reactions
[51]	2013	to model a representative UCG process	3D, no chemical reactions
[52]	2013	to model cavity growth	3D, small-scale dimension (3 × 1.5 × 2 cm), with homogeneous and heterogeneous reactions
[53]	2014	to understand the hydrodynamics within cavity	3D, considers no temperature effect or chemical reactions
[54]	2014	to model cavity growth	3D, with homogeneous and heterogeneous reactions
[55]	2016	to model cavity growth	3D, for flow parameters

additive processes. The software supports a wide range of grid and porosity models, enabling simulation at both field and laboratory scales. With its comprehensive features and capabilities, STARS is a cutting-edge reservoir simulator that addresses a broad spectrum of thermal and advanced processes in the oil and gas industry.

Owing to the rapid advancement of oil and gas simulators, (e.g., CMG STARS) researchers have successfully adapted the reservoir simulator for modelling the UCG process. As shown in Table 5, the main advantage of the CMG software is that it is able to model nearly all the fundamental phenomena involved in UCG in a 3D perspective without a large computational burden. In addition, the hydrocarbon recovery−oriented package exhibits some superior features over other tools, such as complex geology, versatile well layouts, coal ignition and pyrolysis modelling, and flexible injection schemes. Furthermore, CMG owns the package to model the storage of CO_2 in the post-UCG cavities [20,21]. Fig. 11 illustrates the temperature distribution in a CMG-based UCG cavity [27], the characteristics of which represent the distinct chemical regions resulting from physiochemical events.

2.2.4. FLAC3D

FLAC3D presents the most effective solution for tackling intricate geotechnical challenges, offering comprehensive 3D analyses of soil, rock, concrete, structural ground support, and groundwater flow. The software's versatility allows for the inclusion of additional options, such as dynamic, creep, thermal, and IMASS analyses, and the creation of user-defined constitutive models to expand its capabilities. With an 'easy-to-use user interface and new interactive tools, constructing and interpreting models is remarkably intuitive and straightforward. This enables FLAC3D to deliver highly accurate simulations of real-world geotechnical conditions, making it ideal for engineering applications like assessing slope stability, analyzing underground excavation behavior, and simulating earthquake scenarios. To enhance user control and efficiency, FLAC3D provides flexible commands and scripting capabilities, empowering users to parameterize, customize, and automate model processes according to their specific needs. Overall, FLAC3D stands as the foremost choice for addressing complex geotechnical problems and delivering precise engineering insights.

The success of FLAC3D in modelling geotechnical problems has made it a professional tool in the investigation of the geomechanical responses in the context of UCG (see Table 6). As shown by Table 6, the inability of FLAC3D to perform gasification modelling means it must be coupled with other software packages with embedded chemical reaction functions (i.e., CMG, COMSOL Multiphysics and Ansys Fluent). Alternatively, to overcome the limitations of FLAC3D, some

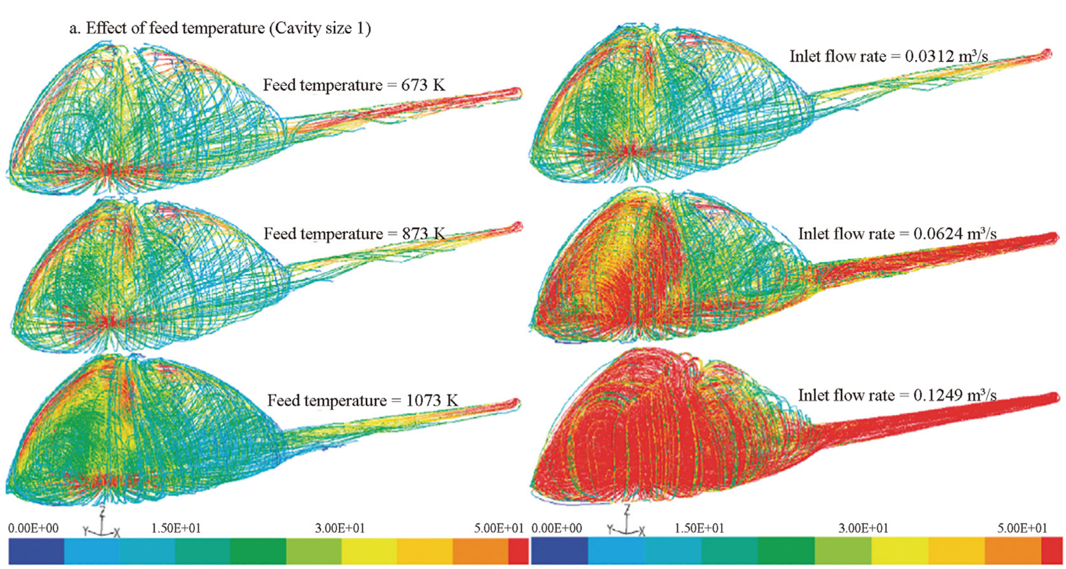

Fig. 10. Velocity lines in the cavity from Ansys Fluent [50].

Table 5
Underground coal gasification investigations with CMG reservoir simulator.

Ref	Year	Objective	Model feature
[56]	2010	feasibility study of using CMG to model UCG	3D, large-scale, with heat and mass transfer, chemical reactions and geology
[57]	2011	to model the CRIP method of UCG	3D, large-scale, with heat and mass transfer, chemical reactions
[58]	2012	to elucidate the methodology to model UCG with CMG	3D, large-scale, with heat and mass transfer, chemical reactions and geology
[59]	2013	to present a method for the estimation of chemical reaction kinetics at high-pressure	3D, large-scale, with heat and mass transfer, chemical kinetics and geology
[60]	2014	to model UCG for import to FLAC3D	3D, large-scale, with heat and mass transfer, chemical kinetics and geology
[61]	2015	to compare three CRIP methods	3D, large-scale, with heat and mass transfer, chemical kinetics and geology
[62]	2016	to model UCG for import to CGG GEOSIM	3D, large-scale, with heat and mass transfer, chemical kinetics
[63]	2017	to model UCG for import to FLAC3D	3D, large-scale, with heat and mass transfer, chemical kinetics and geology
[64]	2017	to model UCG for import to CGG GEOSIM	3D, large-scale, with heat and mass transfer, chemical kinetics
[8]	2017	to model reverse combustion linking in UCG	3D, large-scale, with heat and mass transfer, chemical kinetics
[9]	2018	to model the impact of cleats network	3D, large-scale, with heat and mass transfer, chemical kinetics and geology
[13]	2019	to model UCG with heavy oil mobilization	3D, large-scale, with heat and mass transfer, chemical kinetics and geology
[17]	2019	to model coal pore variations in UCG	3D, large-scale, with heat and mass transfer, chemical kinetics
[27]	2022	to model a new method for deep UCG	3D, large-scale, with heat and mass transfer, chemical kinetics and geology

researchers have used a heating source to probe the thermo-mechanical effects associated with UCG. However, this simplification may underestimate the complexity of the problem, for example, by completely ignoring mass and heat coupling in the chemical reactions. An example of predicted subsidence in a multidimensional perspective is provided in Fig. 12. The growing environmental interest in UCG will result in an increase in the application of FLAC3D in modelling thermal–hydro–chemical–mechanical problems, albeit coupled with other simulators.

2.2.5. MODFLOW

MODFLOW represents the U.S. Geological Survey's modular finite-difference flow model, serving as a computer code designed to solve the groundwater flow equation. Hydrogeologists rely on this program to simulate the movement of groundwater within aquifers. The source code of MODFLOW is freely available as public domain software, predominantly written in Fortran, and is capable of compilation and execution on both Microsoft Windows and Unix-like operating systems.

Table 7 shows that the use of MODFLOW in the context of UCG has been exclusively for modelling groundwater flow under thermo-mechanical effects (e.g., thermally induced fractures in the vicinity of the cavity and in the caprock). The limitations in the modelling capability of MODFLOW in the areas out of groundwater flow indicate an unlikely widespread use in UCG modelling. For instance, CMG would be more suitable in modelling UCG with groundwater flow considerations, without being coupled with other tools.

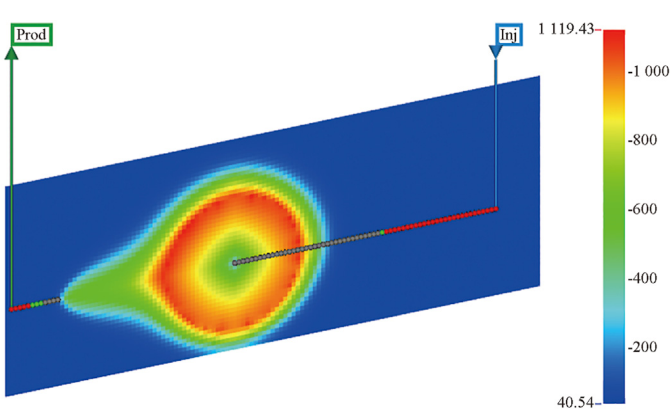

Fig. 11. The temperature profile in an underground coal gasification cavity from CMG modelling [27].

2.2.6. Others

There are other modelling tools for UCG simulations. However, because of partial modelling capabilities or proprietary constraints, they are not commonly used in UCG modelling. For example, as a world pioneer in leading the research in UCG, Lawrence Livermore National Laboratory

Table 6
FLAC3D supported underground coal gasification research.

Ref	Year	Objective	Model feature
[65]	2013	investigating the applicability of UCG in a Bulgarian coal	2D, heat source instead of chemical reactions
[66]	2014	to model stress and deformation	3D, gasification model from CMG
[67]	2015	to predict surface subsidence	3D, includes no UCG gasification
[68]	2015	to study the thermo-mechanical effects on caprock permeability	2D, includes no UCG gasification
[69]	2016	to predict surface subsidence and fault reactivation	3D, includes no UCG gasification
[38]	2016	to model fracture field in the overburden	2D, heat profile from COMSOL
[39]	2017	to model fracture field in caprock	2D, heat profile from COMSOL
[70]	2018	to simulate ground subsidence and mechanical properties degradation	3D, includes no UCG gasification
[71]	2018	to predict surface subsidence	2D, includes no UCG gasification
[72]	2019	to study fracture development and surface subsidence	3D, heat profile from Ansys Fluent
[73]	2020	to predict surface subsidence	3D, heat profile from Ansys Fluent

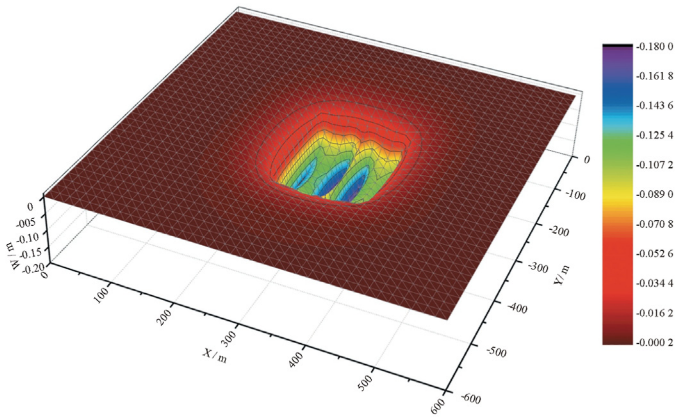

Fig. 12. FLAC3D predicted subsidence in a 3D domain [73].

developed an in-house new integrated 3D UCG Simulator [77–79]; however, the proprietary status of this simulator prevents it from widespread use by global UCG researchers.

UCG modelling studies with RFPA and ABAQUS are rare [80–82]. The possible reasons are that they are costly to access/start with, or because substitutes are easily available to modellers.

3. Challenges and prospect

UCG is a promising low-carbon coal technology and holds the potential to decarbonize the use of coal and mitigate climate change. However, the complex physiochemical events involved in UCG mean that the process is difficult to manage. To optimize performance and reduce or eliminate the environmental concerns associated with UCG, in addition to laboratory- and pilot-scale experiments, substantial modelling endeavors are required.

The daunting task of modelling UCG on a large scale requires the selection of a sound tool. This manuscript provides an overview of the available and accessible numerical tools for modelling UCG. Although a single software package to perform all modelling tasks is presently unavailable, the analysis in this manuscript indicates that many modelling tools are able to explore different aspects of UCG. CMG STARS appears to be the most suitable tool for UCG modelling because it is able to simulate the important aspects pertaining to UCG. However, researchers have the discretion to resort to a suitable software package based on their concrete needs and interests.

While the coupling of different tools is likely to be an effective short-term solution, dedicated work from mathematicians and software developers is required to further enhance the UCG modelling capabilities of the tools. More groundbreaking progress will be achieved if modellers focus on the unresolved problems facing the commercialization of UCG, rather than determining how to best couple various tools together. With coordinated efforts from world researchers, the next 10–15 years will see the development of UCG for substantive commercial operations.

Table 7
Several underground coal gasification studies with MODFLOW application.

Ref	Year	Objective	Model feature
[74]	2004	to study groundwater flow in the context of UCG	3D, regional hydrology modelling
[75]	2016	to explore the feasibility of UCG with CO_2 storage in Bulgaria	3D, regional groundwater model
[76]	2016	to study groundwater flow with induced fractures in UCG	3D, groundwater model
[31]	2017	to study groundwater flow with induced fractures in UCG	3D, groundwater model

Conflict of interest

The authors declare that there is no conflicts of interest.

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