TSCFA台灣超臨界流體協會
Taiwan Supercritical Fluid Association

電子報第 200 期

活動訊息

- **製藥製程減碳新契機：超臨界CO_2在醫藥原料純化與微粒設計之應用工作坊**
  日期：**113年2月2日(五)**
  地點：台北科技大學化學工程館101會議室
  報名網址：https://docs.google.com/forms/d/e/1FAIpQLSft3TewjquMMJmZVG-s3fw-szzxgDZuaQkRupHXp_Rp4Rx4_w/viewform
- ***14 TH ISSF(International Symposium on Supercritical Fluids)***
  日期：**JUNE 2025**
  地點：BALI
  CHAIR：JAEHOON KIM, SOUTH KOREA
  Scientific Meetings – ISASF (supercriticalfluidsociety.net)
- ***19 TH ISSF, (European Meeting on Supercritical Fluids EMSF)***
  日期：**26-29 MAY 2024**
  地點：MARIBOR, SLOVENIA
  CHAIR：ZELJKO KNEZ, SLOVENIA
  Scientific Meetings – ISASF (supercriticalfluidsociety.net)
- ***NEXT AEROGEL MEETING***
  日期：**18 – 20 September 2024**
  地點：Hamburg, Germany
  CHAIR：Irina Smirnova
  http://www.aerogel.org/community/news/

會員動態

- 賀本會邱永和常務監事榮獲『2023 第十九屆 IIP 國際傑出發明家獎-2023 達文西國際創新科技獎』！
- 日本化學工學會超臨界流體來訪
- 徵才活動—綠茵生技股份有限公司

產業新聞

- 體積小效率高，美國超臨界二氧化碳試驗電廠 2024 開始運作
  資料來源：https://technews.tw/2023/11/08/supercritical-transformational-electric-power/

- 世界第一具 CO_2 超臨界渦輪機 僅桌子大 功率就有 1 千萬瓦
  資料來源：https://www.chinatimes.com/realtimenews/20231102005721-260408?chdtv

淨零永續

- ***推動碳中和人才認證班***--混成(實體+線上同步)
  日期：**10/17~12/26，共計58小時**
  地點：台北BR6科技大樓
  https://college.itri.org.tw/edm/D3/009/03/edm.html
  https://college.itri.org.tw/Home/LessonData/FC37461B-8C73-405A-B86C-B6614A82630A?from_rec=recapi-7fd64848bf-77hfp_original_1693576711_2266147
- ***推動碳中和人才認證班-碳交易x碳盤查x碳模式盤點與綠電導入***
  日期：**10/13(五)、10/17(二)、10/20(五)、11/28(二)、12/26(二)**
  地點：實體/線上
  https://college.itri.org.tw/edm/D3/009/03/edm.html
- ***化學產業淨零永續專業推動人才認證班(第03期)新竹***--混成(實體+線上同步)
  日期：**2023/11/30~2024/1/4，共計36小時**
  地點：數位自學雲端教室
  https://college.itri.org.tw/Home/LessonData/2B2E5236-3833-493D-85FD-C6D363C8DE48?from_rec=recapi-7fd64848bf-77hfp_original_1693576726_2266185

◆ IDB 產業節能減碳資訊網 INDUSTRIAL ENERGY SAVING AND CARBON REDUCTION INFORMATION WEB https://ghg.tgpf.org.tw/	◆ 淨零永續學校 https://college.itri.org.tw/nzschool/

團體會員介紹

- 歐境企業股份有限公司

教育訓練班

- (夜間班)高壓氣體特定設備操作人員安全衛生教育訓練班 12/12~12/24
- (日間班)高壓氣體特定設備操作人員安全衛生教育訓練班 12/18~12/22

技術文摘

- An Experimental Investigation of Supercritical Methane Injection Characteristics in a CO_2 Environment CO_2 環境 下超臨界甲烷注入特性實驗研究
- Chemistry and Dynamics of Supercritical Carbon Dioxide and Methane in the Slit Pores of Layered Silicates 層狀矽酸鹽狹縫孔中超臨界二氧化碳和甲烷的化學和動力學

- Direct Numerical Simulation of Fluid Flow and Heat Transfer of a Reactive Particle Layer with Stefan Flow in Supercritical Water 超臨界水中斯特凡流流體流動和反應顆粒層熱傳的直接數值模擬
- Holding water in a sieve—stable droplets without surface tension 將水保持在篩子中－穩定的水滴，沒有表面張力
- Quantification of coumarins, furocoumarins and polymethoxyflavones in hydroalcoholic fragrances by supercritical fluid chromatography-tandem mass spectrometry 超臨界流體層析-串聯質譜法定量水醇香料中的香豆素、呋喃香豆素和多甲氧基黃酮
- Regular Solution Approach to Modeling the Supercritical Fluid Extraction of Two-Component Solutes from Ground Oilseeds 模擬超臨界流體從磨碎的油籽中提取雙組分溶質的常規求解方法
- Supercritical Carbon Dioxide Shock Behavior Near the Critical Point 臨界點附近的超臨界二氧化碳衝擊行為

台灣超臨界流體協會
電話：(07)355-5706　E-mail：tscfa@mail.mirdc.org.tw

製藥製程減碳新契機: 超臨界 CO_2 在醫藥原料純化與微粒設計之應用

在製藥產業的製程設計與開發過程當中，透過使用 CO_2 取代有機溶劑，是另一種可以達到製程減碳的手段之一。近年的學術研究與產業應用方面，超臨界 CO_2 已經被應用於諸多製藥的程序當中，如果進一步搭配成熟的 CO_2 回收技術，將可以更有效地達成減碳的目的。本工作坊，將邀請專家學者，針對如何利用超臨界 CO_2 進行醫藥中間體的純化，以及中後段的微粒製備與製劑設計等進行介紹，以促進產學研的交流，同時拓展超臨界流體在醫藥產業的新契機。

時間：2024 年 2 月 2 日 (五)

地點：台北科技大學化學工程館 101 會議室

報名費：

- 會員: 1,500 元
- 非會員: 2,500 元
- 學生: 1,000 元

議程：

時間	議程	講員
09:00~09:30	報 到	
09:30~09:40	引 言	台灣超臨界流體協會 梁明在理事長
09:40~10:40	超臨界流體層析原理與 API 純化應用	喬璞科技有限公司 包曉青經理
10:40~11:00	茶 歇	
11:00~12:00	超臨界流體模擬移動床層析技術與設備導覽	喬璞科技有限公司 包曉青經理
12:00~13:30	午 餐	
13:30~14:30	超臨界流體技術在肺部釋放藥物製劑之應用	明志科技大學 吳弦聰教授
14:30~14:50	茶 歇	
14:50~15:50	超臨界 CO_2 在 API 固態物性控制、共晶製備與非晶型固體分散微粒設計之應用	台北科技大學 蘇至善教授
15:50~16:20	綜合座談	

主辦單位

台灣超臨界流體協會

協辦單位

臺北科技大學化學工程與生物科技系

臺北科技大學專利暨技術轉移中心

交通方式:

1. 抵達臺北科技大學

搭乘捷運

藍線【板南土城線】忠孝新生站或橘線【中和新蘆線】忠孝新生站，4 號出口台北科技大學。

搭乘公車

【台北科技大學站】: 212、212 直達車、232、262、299 及 605。

【忠孝新生路口站】: 72、109、115、214、222、226、280、290、505、642、665、668、672 及松江新生幹線。

搭乘火車或高鐵

由台北火車站或高鐵台北站直接轉捷運【板南線】至忠孝新生站，4 號出口台北科技大學。

自行開車

【國道一號】: 於建國北路/松江路交流道下(靠左走建國北路高架橋)於忠孝東路出口下(循右線右轉忠孝東路)續行約 100 公尺即達本校。

【國道三號】: 於新店交流道接木柵交流道下辛亥路轉建國南路直走至忠孝東路口即達

※ (由於校內空間有限，恕無法提供停車位，請於學校周邊停車場停車後前來)

2. 校園導覽圖

報名網址：

https://docs.google.com/forms/d/e/1FAIpQLSft3TewjquMMJmZVG-s3fw-szzxgDZuaQkRupHXp_Rp4Rx4_w/viewform

聯絡人

台灣超臨界流體協會 吳家瑩秘書
E-mail: tscfa@mail.mirdc.org.tw Tel: (07)355-5706

賀本會邱永和常務監事榮獲『2023 第十九屆 IIP 國際傑出發明家獎-2023 達文西國際創新科技獎』！

資料來源：https://www.tw580.org/m/412-1296-13186.php

日本化學工學會超臨界流體來訪

日本化學工學會超臨界流體部會長渡邊教授(同時也是東北大學超臨界研究中心主任)，於 11 月 28-30 日領團來台參訪，感謝會員廠家協助相關參訪行程，行程圓滿順利，渡邊教授等成員對台灣的超臨界產業發展讚賞有佳，希望能與台灣在超臨界相關領域有進一步交流合作。






綠茵生技 GREENYN BIOTECHNOLOGY

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研發人員

Job Description

- 保健食品原料R&D，新品專案提報與執行。
- 最適製程開發與試產導入。
- 功效試驗設計&執行、機制分析&驗證。
- 檢驗分析方法開發&確效。
- 市場趨勢分析&資料建立。

Job Conditions

- 具動植物萃取、分析方法與產線製程開發經驗者佳，食品、生科相關領域者為優。
- 個性樂觀積極、開朗活潑。

報名請掃描　104人力銀行　公司網頁

Human Resources Department
04-22382867#171 Cherry
cherrychiang@greenyn.com.tw

體積小效率高，美國超臨界二氧化碳試驗電廠 2024 開始運作

作者 Daisy Chuang | 發布日期 2023 年 11 月 08 日

雖然目前全球正朝能源轉型、再生能源發電邁進，但現在汽輪機（steam turbine）仍然是世界供電主力，相關技術也不斷發展中，未來以「超臨界二氧化碳」為介質的渦輪機有望改變市場，便宜、體積更小，效率還高 10%，美國德州示範電廠也已落成。

美國能源部、美國西南研究院（SWRI）、GTI Energy、GE Vernova 10 月底宣布超臨界電廠（Supercritical Transformational Electric Power，STEP）「機械完成（mechanically complete）」，耗資 1.55 億美元的試點電廠現已在聖安東尼奧竣工。

跟一張桌子差不多大的渦輪機發電量卻達 10 MW，可為一萬戶家庭供電。那麼這個超臨界二氧化碳（sCO2）渦輪機是如何運作的呢？當溫度和壓力分別高於約 31 °C 和 74 bar （1,070 psi）時，二氧化碳將達到超臨界狀態，為維持在臨界溫度及臨界壓力以上的二氧化碳流體。

水當然也可以達到超臨界狀態，只是需要耗費更多的能量，溫度跟壓力需要超過 373 °C 和 220 bar（3,191 psi）。科學家看好超臨界二氧化碳流體的特性，認為這是封閉系統（closed-loop system）中理想的能量提取選擇。

早在 2016 年，GE 就宣布開始建造試點工廠，以證明商用可行性，預計發電量可達 10 MW 熱電轉換效率為 50%，比目前 40 年代中期開始運行的蒸汽渦輪機高出約 10%，而新型渦輪機尺寸也只有十分之一。

如果成功，較小的渦輪機不僅更便宜，所需土地面積更少，單位發電量還能更高，

最重要的是，啟動和開機速度會更快。GE 的原型機運行溫度為 700 °C，只需兩分鐘即可發電，而傳統蒸汽渦輪機則需要至少半小時，因此未來更快速響應電網需求。

一旦經過驗證，未來就有機會擴展到公用事業規模，並取代傳統發電廠的蒸汽渦輪機，只是目前還有許多前置作業，預計將於 2024 年開始運作。

資料來源：https://technews.tw/2023/11/08/supercritical-transformational-electric-power/

世界第一具 CO_2 超臨界渦輪機 僅桌子大 功率就有 1 千萬瓦

2023/11/02　中時新聞網

10 月 27 日，美國能源部、西南研究院 (SWRI)、GTI 能量 (GTI Energy)、奇異-維諾瓦(GE Vernova)共同舉行超臨界轉型電力 (STEP) 示範工廠的開幕剪綵，特別介紹工廠的核心機-「超臨界二氧化碳渦輪機」，它體積只有桌子那麼大，卻有著 10 百萬瓦的大功率，假如運轉成功，將是熱力渦輪機的巨大革命。

新阿特拉斯(New Altas)報導，蒸汽渦輪機應用在大型發電廠裡，包括燃煤火力電廠、燃氣火力電廠、核能發電廠，其原理都是強大的熱力帶動蒸氣渦輪，再由渦輪機轉動發電機。

為了增加效率，工程師開發出「超臨界渦輪機」的構想，超臨界是指超臨界流體，會具有更好流動性。水當然也可以達到超臨界狀態，只要加熱超過 373 度， 壓力 220bar(約 217 倍大氣壓)，就可達到超臨界狀態，當然這需要更多的能量。

西南研究所提出的是以二氧化碳為介質的氣體式渦輪機，由於氣體可以被壓縮，所以渦輪機尺才可以更小，效率也更高。在聖安東尼奧完成的這具示範渦輪機，體積比同功率的蒸氣渦輪機小了 10 倍，但是熱效率卻高了 10%。根據新聞稿，這具耗資 1.55 億美元的世界上第一台超臨界二氧化碳渦輪機，只有一張桌子那麼大，功率卻有 10 百萬瓦，相當於為大約 1 萬戶家庭供電。根據二氧化碳的特性，當溫度達到 31 度，壓力達到 74 bar (約 73 倍大氣壓) 時，二氧化碳就會達到超臨界狀態，比水要來的更容易。

較小的渦輪機不僅更便宜，而且結構緊湊，建造發電廠所需的土地更少。而且它的啟動效率還超級快，只需要 2 分鐘就能開始運轉，如果是蒸氣渦輪機，則需要 30 分鐘。因此它具有快升快降的特性，使其在可再生能源電網中更加有用。

一旦經過驗證，該技術可以擴展到商業與公共建設規模，並開始取代現有發電廠內的的蒸汽渦輪機。舊有的核電廠、地熱電廠、聚光太陽能電的效率都會提高 10 倍以上。

資料來源：https://www.chinatimes.com/realtimenews/20231102005721-260408?chdtv

歐境企業股份有限公司

DETER ENTER PRISE CO., LTD

關於歐境

歐境企業股份有限公司成立於 1988 年，專業領域為**空壓自動化零件進口及研發與製造，尤其在空油配合交互運用的範疇**，如增壓缸、增壓器、增壓泵浦、穩速缸、空油轉換穩速筒、高壓電磁閥、特殊閥類與缸類等。

最大的特色是有足夠的能力配合有潛力的客戶開發有潛力的產品使模組化。協助客戶創造其產品差異化，並提高市場競爭力以提升其產品品質及利潤是歐境一致的目標。

主要商品/服務項目

- 增壓系列：增壓缸、增壓器、氣體增壓泵浦、液體增壓泵浦
- 氣體配重：高壓氣體配重系統、配重缸、主軸式增壓器、直壓式打刀缸、高壓儲氣瓶
- 閥系列：電磁閥、ISO 電磁閥、高壓電磁閥、急速排氣閥、逆止或閥、高壓調壓閥、精密調速閥、針閥
- 缸系列：氣壓缸、油壓缸、配重缸、薄型油壓缸
- 代理產品：義大利 Stampotecnica AirComp、義大利 Bonesi Pneumatic、法製 Asco / Joucomatic、法製 Legris

	流體加壓單元 水壓加壓至 3000kg/cm^2
	空氣加壓系統 5kg/cm^2 加壓至 500kg/cm^2

https://www.deter.com.tw/zh/product.html / 電話：04-22700585

TSCFA 台灣超臨界流體協會
Taiwan Supercritical Fluid Association

(夜間班)高壓氣體特定設備操作人員安全衛生教育訓練班

需要有操作證照的單位，歡迎向協會報名。

●上課日期：**(夜班)112/12/12~12/21 18:30~21:30；12/23~12/24 08:00~17:00(實習)**

●上課時數：高壓氣體特定設備操作人員安全衛生教育訓練課程時數 35 小時＋2 小時(測驗)。

●課程內容：高壓氣體概論 3HR、種類及構造 3HR、附屬裝置及附屬品 3HR、自動檢查與檢點維護 3HR、安全裝置及其使用 3HR、操作要領與異常處理 3HR、事故預防與處置 3HR、安全運轉實習 12HR、高壓氣體特定設備相關法規 2HR，共 35 小時。(另加學科測驗 1 小時及術科測驗約 1~2 小時)

●上課地點：高雄市楠梓區高楠公路 1001 號【金屬工業研究發展中心研發大樓 2 樓　產業人力發展組】

●參加對象：從事高壓氣體特定設備操作人員或主管人員。

●費　　用：本班研習費**新台幣 7,000 元整**，**本會會員享九折優惠**。

●名　　額：每班 30 名，額滿為止。

●結訓資格：期滿經測驗成績合格者，取得【高壓氣體特定設備操作人員安全衛生訓練】之證書。

●報名辦法：1.傳真報名：(07)355-7586台灣超臨界流體協會
2.報名信箱：tscfa@mail.mirdc.org.tw
3.研習費請電匯至 兆豐國際商銀 港都分行(代碼017)
戶名：社團法人台灣超臨界流體協會 帳號：002-09-018479（註明參加班別及服務單位）或以劃線支票抬頭寫「台灣超臨界流體協會」連同報名表掛號郵寄台灣超臨界流體協會，本會於收款後立即開收據寄回。

※洽詢電話：(07)355-5706 吳小姐繳交一吋相片一張及身份證正本

報　　名　　表

課程名稱	高壓氣體特定設備操作人員安全衛生教育訓練			上課日期	112 年 12/12~12/24	
姓　　名	出生年月日	身份證字號	手機號碼	畢業校名		公司產品
服務單位					電　　話	
服務地址	□□□				傳　　真	
發票住址	□□□				統一編號	
負 責 人	人	訓練聯絡人 / 職稱		email：		
參加費用	共　　元	參加性質		□公司指派　　□自行參加		
繳費方式	□郵政劃撥　□支票　□附送現金			報名日期	年　　月　　日	

※ 出生年月日、身份證字號、畢業校名、電話、地址須詳填，以利製作證書。

上課日期時間表

課程名稱：(日間班)高壓氣體特定設備操作人員安全衛生教育訓練班

2023/12/12 (二)	18:30 ~ 21:30
2023/12/13 (三)	18:30 ~ 21:30
2023/12/14 (四)	18:30 ~ 21:30
2023/12/15 (五)	18:30 ~ 21:30
2023/12/18 (一)	18:30 ~ 21:30
2023/12/19 (二)	18:30 ~ 21:30
2023/12/20 (三)	18:30 ~ 21:30
2023/12/21 (四)	18:30 ~ 21:30
2023/12/23 (六)	08:00 ~ 17:00 (實習第 1 組)
2023/12/24 (日)	08:00 ~ 14:00 (實習第 1 組)

TSCFA台灣超臨界流體協會
Taiwan Supercritical Fluid Association

(日間班)高壓氣體特定設備操作人員安全衛生教育訓練班

需要有操作證照的單位，歡迎向協會報名。

●上課日期：**112/12/18~12/20 08:00~17:00；12/21~12/22 08:00~17:00(實習)**

●上課時數：高壓氣體特定設備操作人員安全衛生教育訓練課程時數 35 小時＋2 小時(測驗)。

●課程內容：高壓氣體概論 3HR、種類及構造 3HR、附屬裝置及附屬品 3HR、自動檢查與檢點維護 3HR、安全裝置及其使用 3HR、操作要領與異常處理 3HR、事故預防與處置 3HR、安全運轉實習 12HR、高壓氣體特定設備相關法規 2HR，共 35 小時。(另加學科測驗 1 小時及術科測驗約 1~2 小時)

●上課地點：高雄市楠梓區高楠公路 1001 號【金屬工業研究發展中心研發大樓 2 樓　產業人力發展組】

●參加對象：從事高壓氣體特定設備操作人員或主管人員。

●費　　用：本班研習費**新台幣 7,000 元整**，**本會會員享九折優惠**。

●名　　額：每班 30 名，額滿為止。

●結訓資格：期滿經測驗成績合格者，取得【高壓氣體特定設備操作人員安全衛生訓練】之證書。

●報名辦法：1.傳真報名：(07)355-7586台灣超臨界流體協會
2.報名信箱：tscfa@mail.mirdc.org.tw
3.研習費請電匯至 兆豐國際商銀 港都分行(代碼017)
戶名：社團法人台灣超臨界流體協會 帳號：002-09-018479（註明參加班別及服務單位）或以劃線支票抬頭寫「台灣超臨界流體協會」連同報名表掛號郵寄台灣超臨界流體協會，本會於收款後立即開收據寄回。

※洽詢電話：(07)355-5706 吳小姐繳交一吋相片一張及身份證正本

報　　名　　表

課程名稱	高壓氣體特定設備操作人員安全衛生教育訓練			上課日期	112 年 12/18~12/22	
姓　　名	出生年月日	身份證字號	手機號碼	畢業校名		公司產品
服務單位				電　　話		
服務地址	□□□			傳　　真		
發票住址	□□□			統一編號		
負 責 人	人	訓練聯絡人 / 職稱		email：		
參加費用	共　　元	參加性質		□公司指派	□自行參加	
繳費方式	□郵政劃撥　□支票　□附送現金			報名日期	年　月　日	

※ 出生年月日、身份證字號、畢業校名、電話、地址須詳填，以利製作證書。

上課日期時間表

課程名稱：(日間班)高壓氣體特定設備操作人員安全衛生教育訓練班

2023/12/18 (一)	08:00 ~ 17:00
2023/12/19 (二)	08:00 ~ 17:00
2023/12/20 (三)	08:00 ~ 17:00
2023/12/21 (四)	08:00 ~ 17:00 (實習第 1 組)
2023/12/22 (五)	08:00 ~ 14:00 (實習第 1 組)

An Experimental Investigation of Supercritical Methane Injection Characteristics in a CO_2 Environment

CO_2 環境 下超臨界甲烷注入特性實驗研究

By **Ritesh Ghorpade, Gihun Kim, K. R. V. Manikantachari (Raghu), Joshua Weiner, Daniel T. Banuti, Subith Vasu**

Center for Advanced Turbomachinery and Energy Research (CATER), University of Central Florida, Orlando, FL 32816

Abstract

Clean energy generation is gaining significant attention from industries, academia, and governments across the globe. The Allam cycle is one such technology that has been under focus due to its efficiency, environmental friendliness, and economics. This is a direct-fired cycle operating at supercritical conditions using carbon dioxide as a working fluid. Fuel or oxidizer jet mixing with CO_2 is a vital phenomenon that governs combustion efficiency, and it is not well understood for the Allam cycle conditions. This paper experimentally investigated the jet characteristics of a methane jet injected into a subcritical to supercritical carbon dioxide environment. A wide range of injection pressures and temperatures were targeted between subcritical to supercritical conditions. Unlike previous studies, the current work focused on injecting lower-density (methane) jets into higher-density (carbon dioxide) environments. Schlieren imaging and methane absorption measurements were simultaneously performed with a CMOS high-speed camera and a 3.39 μm infrared laser. Specifically, we looked at the classical injection parameter of jet spreading angle, which was classically established to be mainly a density ratio function. Here, the jet cone angle was obtained from the postprocessed schlieren imaging. The jet cone angle is a critical characteristic parameter that describes the entrainment rate in a jet; thus, it is a crucial parameter in understanding the nature of the jet. The laser measurements were only used as an additional check to confirm the entry time of methane into the chamber filled with carbon dioxide. Notably, this paper makes a detailed comparison between the jet cone angles of jets with a density ratio. The result showed that the classical correlations, such as Abramovich's theory applied to submerged turbulent gas jets developed for low-density ratio jets, were unsuitable for higher-density ratio jets. It was also observed that the divergence angles were dependent not only on density ratio but also on other parameters such as pressure ratios and reduced pressures.

Keywords: jet spreading, supercritical CO_2, methane injection, subcritical region

資料來源：https://doi.org/10.1115/1.4055632

Chemistry and Dynamics of Supercritical Carbon Dioxide and Methane in the Slit Pores of Layered Silicates

層狀矽酸鹽狹縫孔中超臨界二氧化碳和甲烷的化學和動力學

By **Geoffrey M. Bowers*, Narasimhan Loganathan, John S. Loring, Herbert Todd Schaef, and A. Ozgur Yazaydin**

Department of Chemical Engineering, University College London, London, U.K. WC1E 7JE

Abstract

Conspectus

In the mid 2010s, high-pressure diffraction and spectroscopic tools opened a window into the molecular-scale behavior of fluids under the conditions of many CO_2 sequestration and shale/tight gas reservoirs, conditions where CO_2 and CH4 are present as variably wet supercritical fluids. Integrating high-pressure spectroscopy and diffraction with molecular modeling has revealed much about the ways that supercritical CO_2 and CH4 behave in reservoir components, particularly in the slit-shaped micro- and mesopores of layered silicates (phyllosilicates) abundant in caprocks and shales. This Account summarizes how supercritical CO_2 and CH4 behave in the slit pores of swelling phyllosilicates as functions of the H_2O activity, framework structural features, and charge-balancing cation properties at 90 bar and 323 K, conditions similar to a reservoir at ∼1 km depth. Slit pores containing cations with large radii, low hydration energy, and large polarizability readily interact with CO_2, allowing CO_2 and H_2O to adsorb and coexist in these interlayer pores over a wide range of fluid humidities. In contrast, cations with small radii, high hydration energy, and low polarizability weakly interact with CO_2, leading to reduced CO_2 uptake and a tendency to exclude CO_2 from interlayers when H_2O is abundant. The reorientation dynamics of confined CO_2 depends on the interlayer pore height, which is strongly influenced by the cation properties, framework properties, and fluid humidity. The silicate structural framework also influences CO_2 uptake and behavior; for example, smectites with increasing F-for-OH substitution in the framework take up greater quantities of CO_2. Reactions that trap CO_2 in carbonate phases have been observed in thin H_2O films near smectite surfaces, including a dissolution–reprecipitation mechanism when the edge surface area is large and an ion exchange–precipitation mechanism when the interlayer cation can form a highly insoluble carbonate. In contrast, supercritical CH_4 does not readily associate with cations, does not react with smectites, and is only incorporated into interlayer slit mesopores when

(i) the pore has a z-dimension large enough to accommodate CH_4, (ii) the smectite has low charge, and (iii) the H_2O activity is low. The adsorption and displacement of CH_4 by CO_2 and vice versa have been studied on the molecular scale in one shale, but opportunities remain to examine behavioral details in this more complicated, slit-pore inclusive system.

資料來源：https://doi.org/10.1021/acs.accounts.3c00188

Direct Numerical Simulation of Fluid Flow and Heat Transfer of a Reactive Particle Layer with Stefan Flow in Supercritical Water

超臨界水中斯特凡流流體流動和反應顆粒層熱傳的直接數值模擬

By **Yingdong Wang, , and Hui Jin***

State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an710049, China

Abstract

Supercritical water gasification is an efficient and clean way of energy conversion. The research on different scales, such as the system, reactor, and particle, has different temporal and spatial significance. A study on particle–particle and particle–fluid–particle interaction on the particle scale has a fundamental guiding value for revealing gasification performance on the reactor scale. Reactive particles such as coal are pyrolyzed and gasified in a high-temperature and high-pressure reactor to form Stefan flow, which affects the mass, momentum, and energy transfer between particles and supercritical water. In this paper, a particle-resolved direct numerical simulation study of a reactive particle layer in supercritical water is carried out to investigate the effect of different particle layer solid holdups and Stefan flow intensities and distributions on the flow and heat transfer process between the particle layer and supercritical water. This work analyzes the pressure and friction drag coefficients to which the particles are subjected and specifies the flow, velocity, and temperature distribution inside and around the particle layer. The results show that the drag coefficient and Nusselt number of particles in the particle layer decrease gradually along the flow direction, and the presence of particle Stefan flow further reduces the drag force and Nusselt number of particles. With the increasing solid holdup of the particle layer, the particle–fluid–particle interaction becomes more intense, and the effect of Stefan flow cannot be negligible.

資料來源：https://doi.org/10.1021/acs.iecr.2c03866

Holding water in a sieve—stable droplets without surface tension

將水保持在篩子中 - 穩定的水滴，沒有表面張力

By **N. P. Longmire, S. L. Showalter & D. T. Banuti**

Department of Nuclear Engineering, The University of New Mexico, Albuquerque, NM, 87131, USA

Abstract

Our understanding of supercritical fluids has seen exciting advances over the last decades, often in direct contradiction to established textbook knowledge. Rather than being structureless, we now know that distinct supercritical liquid and gaseous states can be distinguished and that a higher order phase transition - pseudo boiling - occurs between supercritical liquid and gaseous states across the Widom line. Observed droplets and sharp interfaces at supercritical pressures are interpreted as evidence of surface tension due to phase equilibria in mixtures, given the lack of a supercritical liquid-vapor phase equilibrium in pure fluids. However, here we introduce an alternative physical mechanism that unexpectedly causes a sharpening of interfacial density gradients in absence of surface tension: thermal gradient induced interfaces (TGIIF). We show from first principles and simulations that, unlike in gases or liquids, stable droplets, bubbles, and planar interfaces can exist without surface tension. These results challenge and generalize our understanding of what droplets and phase interfaces are, and uncover yet another unexpected behavior of supercritical fluids. TGIIF provide a new physical mechanism that could be used to tailor and optimize fuel injection or heat transfer processes in high-pressure power systems.

資料來源：https://www.nature.com/articles/s41467-023-39211-z

Quantification of coumarins, furocoumarins and polymethoxyflavones in hydroalcoholic fragrances by supercritical fluid chromatography-tandem mass spectrometry

超臨界流體層析-串聯質譜法定量水醇香料中的香豆素、呋喃香豆素和多甲氧基黃酮

By **Marina Russo, Alessandra Trozzi, Luigi Mondello & Paola Dugo**

Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Messina, Italy

Abstract

Citrus essential oils, thanks to their pleasant aroma, are certainly the most used ingredients in the formulation of hydroalcoholic fragrances. The non-volatile fraction of *Citrus* essential oil is composed for 10–20% of coumarins, furocoumarins and polymethoxyflavones. It is well known that furocoumarins induce photosensitization and have potential carcinogenic and mutagenic effects. It follows that furocoumarins levels in cosmetics product are constantly monitored by opinions and regulations issued by the International Fragrance Association.

The aim of this research article was to quantify coumarins, furocoumarins and polymethoxyflavones in thirty commercial hydroalcoholic fragrances using supercritical fluid chromatography in combination with triple quadrupole mass spectrometry technique (SFC-QqQ-MS). According to author's knowledge, this is the first report on the determination of oxygen heterocyclic compounds in hydroalcoholic fragrances by means of SFC-QqQ-MS technique.

Keywords: Furocoumarins, hydroalcoholic fragrances, supercritical fluid chromatography, citrus essential oils, quality control

資料來源：https://doi.org/10.1080/10412905.2023.2236626

Regular Solution Approach to Modeling the Supercritical Fluid Extraction of Two-Component Solutes from Ground Oilseeds

模擬超臨界流體從磨碎的油籽中提取雙組分溶質的常規求解方法

By **Artur A. Salamatin* and Alyona S. Khaliullina**

Institute of Mechanics and Engineering, FRC Kazan Scientific Center, Russian Academy of Sciences, 2/31 Lobachevsky str., Kazan 420111, Russia

Institute of Computational Mathematics and Information Technologies, Kazan Federal University, 18 Kremlyovskaya str., Kazan 420008, Russia

Abstract

The extract obtained at supercritical fluid extraction from plant raw material is essentially multicomponent. A multicomponent mass-transfer model at the particle scale is developed to account for the non-ideality of the chemical interactions between solute components. The oil is represented by two pseudo-components, and the gradient of the chemical potential is considered the driving force for the mass transfer. The model is based on the regular solution and Gibbs energy approaches to the thermodynamic modeling of phase equilibria that take place in the raw material with a high initial oil content. The Stefan–Maxwell approach is used to balance the drag effect/chemical interactions and the driving force of diffusion in a non-equilibrium multicomponent solution. It is demonstrated that the two solute components may act as “co-solvents”, thus facilitating the extraction of each other, or as “anti-solvents”, thus decreasing the overall extraction rates. At least a 60% relative error in the overall flux from the particle surface is observed when the developed model is compared against a simplified approach that considers the solution as an ideal system. It is found that while the flowing fluid accumulates the extracted solute, the phase separation may take place in the pore volume of the packed bed. Possible conditions of phase separation in the pores of the packed bed are discussed.

資料來源：https://doi.org/10.1021/acs.iecr.3c01488

Supercritical Carbon Dioxide Shock Behavior Near the Critical Point

臨界點附近的超臨界二氧化碳衝擊行為

By **Jinhong Wang, Teng Cao, Ricardo Martinez-Botas**

Department of Mechanical Engineering, Imperial College London, London SW7 2AZ, UK

Abstract

This paper aims to provide an understanding of sCO_2 inviscid adiabatic normal shock behavior near the critical point and to develop an explicit tool for faster prediction of the shock relations that can aid the supercritical turbomachinery design process. An iterative algorithm was developed to compute shockwave behaviors for nonideal fluids. Three important shock behavior parameters were investigated: postshock Mach number, shock strength, and polytropic efficiency. A comparative study was carried out between air (ideal gas assumption), ideal gas CO_2 (ideal gas assumption), and nonideal fluid CO_2 (Span–Wagner equation of state). The distinct differences show the inadequacy of the perfect gas shock relations when predicting sCO_2 shock behavior near the critical point. The results of nonideal fluid calculations show a general trend of stronger shock strengths and higher polytropic efficiencies toward lower preshock entropy conditions. This is also distinctive near the critical point due to the reduced speed of sound. Finally, explicit expressions for these parameters were retrieved using symbolic regression. The fitted models have significant improvements compared to the prediction from perfect gas shock relations with a 5–20% point reduction in relative errors. This study also shows the potential for machine learning to be applied in nonideal fluid effects modeling and the methodology developed in this paper can be easily introduced to other working fluids in their ranges of interest.

資料來源： https://doi.org/10.1115/1.4063384