ESA Carbon from Space: Inorganic carbon and air/sea CO_2 flux session synthesis

A number of fundamental priorities were identified during the *Inorganic carbon and air/sea CO_2 fluxes* session. A key overarching challenge is to find an optimal way of combining satellites, models and in situ observations (from ships and autonomous vehicles) to produce best-quality data products. This is critical if we are to:

i) measure and monitor the marine inorganic carbon cycle as part of any near real-time forecasting capability of the biogeochemical ocean carbon cycle; and
ii) apply this information in any regional or global impact assessments to assess the multiple stressors (e.g. temperature change, ocean acidification) acting upon the marine ecosystem and subsequent downstream effects on the carbon cycle, natural food web, fisheries, etc.

Another concern common to all observations of the marine carbon cycle is the limited resource available and how best to use that resource. Current funding levels make it challenging to support adequate monitoring of core ocean carbon variables in addition to supporting innovative blue skies science. Increasing overall funding and separating the funding pots for the two activities could help to maximise monitoring and achieve key priorities for blue skies research.

Below we detail the current capabilities for assessing surface ocean inorganic carbon pools and fluxes. We then list the gaps that can and should be filled through a list of short-medium term objectives.

Current capabilities

Particulate inorganic carbon (PIC) remote sensing has focused on the detection of coccolithophores (Balch et al., 2005; Gordon et al., 2001; Mitchell et al., 2017). Due to their unique optical signature, coccolithophore blooms have been detected via satellite ocean colour since the launch of the Coastal Zone Color Scanner in 1978 (Brown & Yoder, 1994; Holligan et al., 1983). The challenge is to detect coccolithophores and their associated PIC at low concentrations, as well as during bloom events. Laboratory (Voss et al., 1998; Balch et al., 1999) and field (Balch et al., 1996; Smyth et al., 2002) observations have informed PIC algorithm development by relating coccolithophore abundance and morphology to PIC concentrations. Currently NASA Ocean Biology DAAC distributes a PIC product that merges Balch et al. (2005) and Gordon et al. (2001), and there is also a developmental PIC product (Mitchell et al., 2017).

Dissolved inorganic carbon (DIC) and other carbonate system parameters (e.g., total alkalinity, TA, partial pressure of CO_2 in seawater, pCO_2) are more challenging to determine from satellite observations as they don't have a coloured component and are controlled by both physical and biological processes. This has led to the development of regional relationships to predict DIC or TA from salinity (e.g., Cai et al., 2010; Lefévre et al., 2010) and temperature (Lee et al., 2006), as well as global relationships using a suite of physical and chemical parameters (e.g., Sasse et al., 2013). More recently, efforts to combine physical and optical satellite ocean observations with climatological and re-analysis data products has opened the door to remote estimation of the marine carbonate system via regional and global relationships as well as new machine learning methods (e.g., Gregor & Gruber, 2021; Land et al., 2019). Furthermore, modelling studies have been used to evaluate the drivers of the marine carbonate system (Lauderdale et al., 2016) and examine potential impacts of extreme, compound events (Salisbury & Jönsson, 2018; Gruber et al., 2021).

The flux of CO_2 between ocean and atmosphere can be described using a simple equation first described by Liss and Slater (1974): Flux=KΔCO_2; where K is the gas transfer velocity (equivalent to the inverse of the resistance to gas transfer) and ΔCO_2 is the difference between the CO_2 concentrations in the atmosphere and ocean. Ocean temperature influences the partial pressure of CO_2 in seawater and is thus an important determinant of the ΔCO_2. K has typically been parameterised as a function of wind speed (e.g. Wanninkhof et al., 2014).

Large scale air/sea flux estimates typically make use of the global seawater pCO_2 database (SOCAT; Bakker et al., 2016) and/or global climatologies of surface seawater pCO_2 using data interpolation/extrapolation and neural network techniques (e.g. Landschutzer et al., 2020; Takahashi et al., 2009). Climatological seawater pCO_2 fields can be coupled with satellite retrievals of SST, wind speed, etc. to calculate the air-sea CO_2 flux (as demonstrated with the *FluxEngine*: Shutler et al., 2016). Satellite observations have also been combined with model output to estimate pCO_2 and air-sea flux (e.g. Arrigo et al., 2010). Estimates of pCO_2 and air-sea flux have been achieved solely from satellite observations (e.g. Ono et al., 2004; Borges et al., 2009; Lohrenz et al., 2018). It is also possible to calculate seawater pCO_2 from observations of TA and DIC and using a version of *pCO2sys* (e.g. Humphreys et al., 2022).

Seawater pCO_2 and air-sea CO_2 fluxes can also be estimated using models such as ECCO-Darwin (Carroll et al., 2020), which are initialised with a suite of physical variables, biogeochemical properties and also TA, DIC and pCO_2 from datasets such as SOCAT and GLODAP. The advantage of the ECCO-Darwin model is that it assimilates a combination of physical and biogeochemical data in order to produce physically-conserved properties. As such models continue to evolve, it will be increasing possible to use them to assess regional and global scale carbon inventories as well as fluxes.

Gaps and objectives

The gaps in our current capacity for the detection of inorganic carbon and the air-sea flux of CO_2 from space fall into two broad categories: gaps relevant to observing any aspect of the aquatic carbon system (system-wide gaps), and gaps relevant to inorganic carbon and flux products (product-specific gaps).

System-wide gaps:

1. For all components of the inorganic carbon cycle and carbonate system, we lack a measure of the pixel-by-pixel uncertainty on the satellite products.
2. We need greater spatial and temporal coverage of field observations for rigorous development and validation of methods (especially using data-rich, machine learning approaches), including water column observations.
3. Closer collaboration between data generators and modellers is required to improve data assimilation directly into Earth System Models.
4. Ultimately, top-down (e.g., machine learning) and bottom-up (e.g., theoretical understanding of the system) approaches need to be combined to improve satellite products.

Product-specific gaps:

1. Current PIC satellite products are global and are not accurate in environments where other highly scattering materials are present (e.g., coastal shelf seas). There is a lack of coincident in

situ observations of PIC and other highly scattering materials, along with full spectral measurements of specific inherent optical properties for PIC.

2. Sustained, long-term monitoring of seawater pCO_2 and fluxes in key ocean regions (e.g. North Atlantic) is essential, yet there is currently no dedicated framework in place to provide/guarantee these data.
3. Current air-sea CO_2 flux climatologies are spatially and temporally limited by the extent and number of observations. Climatologies are also hampered by how best to extrapolate observations to different SST (both horizontally and to the air-sea interface).
4. Quality assurance of observations. TA/DIC observations require a certified reference material (CRM) and the future availability of this is limited/threatened. Direct air-sea CO_2 flux observations require community-wide agreement on best practice approaches in order to establish a fiducial reference method (FRM) for validation of satellite estimates.
5. Improved process understanding of K needs to focus on understanding relevant and uncertain processes. For example, there is still uncertainty surrounding near surface temperature gradients (see Woolf et al., 2016) and the role of wave breaking, bubbles and turbulence (see Bell et al., 2017; Blomquist et al., 2017).
6. Carbon dynamics and air/sea CO_2 fluxes in mixed sea ice regions are poorly understood (see Watts et al., 2022), which is a major gap in understanding given that climate at the poles is changing rapidly, affecting sea ice melt/freeze processes and timings.

Short/medium-term objectives

- Increase the amount of data from a range of sources (model output, satellite, ships, autonomous platforms) and link them across disciplines (biogeochemical, physical, optical, biological) to produce best quality data products.
- Refine which satellite, model and in situ reanalysis data products to provide accurate, high resolution pCO_2, DIC and TA estimations on local, regional and global scales.
- Reconcile model carbon budgets with both satellite and in situ observations by constraining the different terms within the budget.
- Exploit novel technologies to improve understanding of standing stocks and fluxes in a range of environments (e.g. low winds, high winds, marginal ice zones). For example, gas transfer estimates need to be improved, potentially by exploiting measures other than wind speed (e.g. sea state or sea surface roughness using backscattering observations, see Goddijn-Murphy et al., 2013).
- Generate robust, community-accepted processes and materials to satisfy the necessary CRM and FRM requirements.

References

Arrigo, K. R., Pabi, S., van Dijken, G. L., & Maslowski, W. (2010). Air-sea flux of CO_2 in the Arctic Ocean, 1998–2003. *Journal of Geophysical Research*, *115*(G4), 1998–2003. https://doi.org/10.1029/2009jg001224

Bakker, D. C. E., B. Pfeil, C. S. Landa, N. Metzl, K. M. O'Brien, A. Olsen, K. Smith, C. Cosca, S. Harasawa, S. D. Jones, S. I. Nakaoka, Y. Nojiri, U. Schuster, T. Steinhoff, C. Sweeney, T. Takahashi, B.

Tilbrook, C. Wada, R. Wanninkhof, S. R. Alin, C. F. Balestrini, L. Barbero, N. R. Bates, A. A. Bianchi, F. Bonou, J. Boutin, Y. Bozec, E. F. Burger, W. J. Cai, R. D. Castle, L. Chen, M. Chierici, K. Currie, W. Evans, C. Featherstone, R. A. Feely, A. Fransson, C. Goyet, N. Greenwood, L. Gregor, S. Hankin, N. J. Hardman-Mountford, J. Harlay, J. Hauck, M. Hoppema, M. P. Humphreys, C. W. Hunt, B. Huss, J. S. P. Ibánhez, T. Johannessen, R. Keeling, V. Kitidis, A. Körtzinger, A. Kozyr, E. Krasakopoulou, A. Kuwata, P. Landschützer, S. K. Lauvset, N. Lefèvre, C. Lo Monaco, A. Manke, J. T. Mathis, L. Merlivat, F. J. Millero, P. M. S. Monteiro, D. R. Munro, A. Murata, T. Newberger, A. M. Omar, T. Ono, K. Paterson, D. Pearce, D. Pierrot, L. L. Robbins, S. Saito, J. Salisbury, R. Schlitzer, B. Schneider, R. Schweitzer, R. Sieger, I. Skjelvan, K. F. Sullivan, S. C. Sutherland, A. J. Sutton, K. Tadokoro, M. Telszewski, M. Tuma, S. M. A. C. van Heuven, D. Vandemark, B. Ward, A. J. Watson and S. Xu (2016). "A multi-decade record of high-quality fCO2 data in version 3 of the Surface Ocean CO2 Atlas (SOCAT)." Earth System Science Data 8(2): 383-413.

Balch, W. M., Kilpatrick, K. A., & Trees, C. C. (1996). The 1991 coccolithophore bloom in the central North Atlantic. 1. Optical properties and factor affecting their distribution. *Limnol. Oceanogr.*, *41*(8), 1669–1683.

Balch, W. M., Drapeau, D. T., Cucci, T. L., Vaillancourt, R. D., Kilpatrick, K. A., & Fritz, J. J. (1999). Optical backscattering by calcifying algae: Separating the contribution of particulate inorganic and organic carbon fractions. *Journal of Geophysical Research: Oceans*, *104*(C1), 1541–1558. https://doi.org/10.1029/1998JC900035

Balch, W. M., Gordon, H. R., Bowler, B. C., Drapeau, D. T., & Booth, E. S. (2005). Calcium carbonate measurements in the surface global ocean based on Moderate-Resolution Imaging Spectroradiometer data. *Journal of Geophysical Research C: Oceans*, *110*(7), 1–21. https://doi.org/10.1029/2004JC002560

Bell, T. G., S. Landwehr, S. D. Miller, W. J. de Bruyn, A. H. Callaghan, B. Scanlon, B. Ward, M. Yang and E. S. Saltzman (2017). "Estimation of bubble-mediated air-sea gas exchange from concurrent DMS and CO_2 transfer velocities at intermediate–high wind speeds." Atmos. Chem. Phys. 17(14): 9019-9033.

Blomquist, B. W., S. E. Brumer, C. W. Fairall, B. J. Huebert, C. J. Zappa, I. M. Brooks, M. Yang, L. Bariteau, J. Prytherch, J. E. Hare, H. Czerski, A. Matei and R. W. Pascal (2017). "Wind speed and sea state dependencies of air-sea gas transfer: Results from the High Wind Speed Gas Exchange Study (HiWinGS)." Journal of Geophysical Research: Oceans 122(10): 8034-8062.

Borges, a V., Ruddick, K., Lacroix, G., Nechad, B., Asteroca, R., Rousseau, V., & Harlay, J. (2009). Estimating pCO_2 From Remote Sensing in the Belgian Coastal Zone. *ESA Special Publication SP-686*, (1), 2–7.

Brown, C. W., & Yoder, J. A. (1994). Coccolithophorid blooms in the global ocean. *Journal of Geophysical Research: Oceans*, *99*(C4), 7467–7482. https://doi.org/10.1029/93JC02156

Cai, W.-J., Hu, X., Huang, W.-J., Jiang, L.-Q., Wang, Y., Peng, T.-H., & Zhang, X. (2010). Alkalinity distribution in the western North Atlantic Ocean margins. *Journal of Geophysical Research: Oceans*, *115*(C8). https://doi.org/10.1029/2009JC005482

Carroll, D., D. Menemenlis, J. F. Adkins, K. W. Bowman, H. Brix, S. Dutkiewicz, I. Fenty, M. M. Gierach, C. Hill, O. Jahn, P. Landschützer, J. M. Lauderdale, J. Liu, M. Manizza, J. D. Naviaux, C. Rödenbeck, D. S. Schimel, T. Van der Stocken and H. Zhang (2020). "The ECCO-Darwin data-assimilative global ocean biogeochemistry model: Estimates of seasonal to multidecadal surface ocean pCO2 and air-sea CO2 flux." Journal of Advances in Modeling Earth Systems 12(10): e2019MS001888.

Goddijn-Murphy, L., D. K. Woolf, B. Chapron and P. Queffeulou (2013). "Improvements to estimating the air-sea gas transfer velocity by using dual-frequency, altimeter backscatter." Remote Sensing of Environment 139: 1-5.

Gordon, R., Boynton, G. C., Balch, W. M., Harbour, D. S., Smyth, T. J., & Bay, W. B. (2001). Retrieval of Coccolithophore from SeaWiFS Imagery Calcite Concentration radiance, *28*(8), 1587–1590.

Gregor, L., & Gruber, N. (2021). OceanSODA-ETHZ: a global gridded data set of the surface ocean carbonate system for seasonal to decadal studies of ocean acidification. *Earth System Science Data*, *13*(2), 777–808. https://doi.org/10.5194/essd-13-777-2021

Gruber, N., Boyd, P. W., Frölicher, T. L., & Vogt, M. (2021). Biogeochemical extremes and compound events in the ocean. *Nature*, *600*(7889), 395–407. https://doi.org/10.1038/s41586-021-03981-7

Holligan, P. M., Villior, M., Harbour, D. S., Camus, P., & Champagne-Philippe, M. (1983). Satellite and ship studies of coccolithophore production along a continental shelf edge. *Nature*, *304*, 339–342.

Humphreys, M. P., E. R. Lewis, J. D. Sharp and D. Pierrot (2022). "PyCO2SYS v1.8: marine carbonate system calculations in Python." Geosci. Model Dev. 15(1): 15-43.

Land, P. E., Findlay, H. S., Shutler, J. D., Ashton, I. G. C., Holding, T., Grouazel, A., et al. (2019). Optimum satellite remote sensing of the marine carbonate system using empirical algorithms in the global ocean, the Greater Caribbean, the Amazon Plume and the Bay of Bengal. *Remote Sensing of Environment*, *235*, 111469. https://doi.org/10.1016/j.rse.2019.111469

Landschützer, P., G. G. Laruelle, A. Roobaert and P. Regnier (2020). "A uniform pCO_2 climatology combining open and coastal oceans." Earth Syst. Sci. Data 12(4): 2537-2553.

Lauderdale, J. M., Dutkiewicz, S., Williams, R. G., & Follows, M. J. (2016). Quantifying the drivers of ocean-atmosphere CO2 fluxes. *Global Biogeochemical Cycles*, *30*(7), 983–999. https://doi.org/10.1002/2016GB005400

Liss, P. S. and P. G. Slater (1974). "Flux of gases across the air-sea interface." Nature 247(5438): 181-184.

Lee, K., Tong, L. T., Millero, F. J., Sabine, C. L., Dickson, A. G., Goyet, C., et al. (2006). Global relationships of total alkalinity with salinity and temperature in surface waters of the world's oceans. *Geophysical Research Letters*, *33*(19), 1–5. https://doi.org/10.1029/2006GL027207

Lefévre, N., Diverrés, D., & Gallois, F. (2010). Origin of CO2 undersaturation in the western tropical Atlantic. *Tellus B: Chemical and Physical Meteorology*, *62*(5), 595–607. https://doi.org/10.1111/j.1600-0889.2010.00475.x

Lohrenz, S. E., Cai, W. J., Chakraborty, S., Huang, W. J., Guo, X., He, R., et al. (2018). Satellite estimation of coastal pCO_2 and air-sea flux of carbon dioxide in the northern Gulf of Mexico. *Remote Sensing of Environment*, *207*(January 2017), 71–83. https://doi.org/10.1016/j.rse.2017.12.039

Mitchell, C., Hu, C., Bowler, B., Drapeau, D., & Balch, W. M. (2017). Estimating Particulate Inorganic Carbon Concentrations of the Global Ocean From Ocean Color Measurements Using a Reflectance Difference Approach. *Journal of Geophysical Research: Oceans*, *122*, 8707–8720. https://doi.org/10.1002/2017JC013146

Ono, T., Saino†, T., Kurita, N., & Sasaki, K. (2004). Basin-scale extrapolation of shipboard pCO2 data by using satellite SST and Chla. *International Journal of Remote Sensing*, *25*(19), 3803–3815. https://doi.org/10.1080/01431160310001657515

Salisbury, J. E., & Jönsson, B. F. (2018). Rapid warming and salinity changes in the Gulf of Maine alter surface ocean carbonate parameters and hide ocean acidification. *Biogeochemistry*, *141*(3), 401–418. https://doi.org/10.1007/s10533-018-0505-3

Sasse, T. P., McNeil, B. I., & Abramowitz, G. (2013). A novel method for diagnosing seasonal to inter-annual surface ocean carbon dynamics from bottle data using neural networks. *Biogeosciences*, *10*(6), 4319–4340. https://doi.org/10.5194/bg-10-4319-2013

Shutler, J. D., P. E. Land, J.-F. Piolle, D. K. Woolf, L. Goddijn-Murphy, F. Paul, F. Girard-Ardhuin, B. Chapron and C. J. Donlon (2016). "FluxEngine: A flexible processing system for calculating atmosphere-ocean carbon dioxide gas fluxes and climatologies." Journal of Atmospheric and Oceanic Technology 33(4): 741-756.Smyth, T. J., Moore, G. F., Groom, S. B., Land, P. E., & Tyrrell, T. (2002). Optical modeling and measurements of a coccolithophore bloom. *Applied Optics*, *41*(36), 7679–7688. https://doi.org/10.1364/AO.41.007679

Takahashi, T., S. C. Sutherland, R. Wanninkhof, C. Sweeney, R. A. Feely, D. W. Chipman, B. Hales, G. Friederich, F. Chavez, C. Sabine, A. Watson, D. C. E. Bakker, U. Schuster, N. Metzl, H. Yoshikawa-Inoue, M. Ishii, T. Midorikawa, Y. Nojiri, A. Kortzinger, T. Steinhoff, M. Hoppema, J. Olafsson, T. S. Arnarson, B. Tilbrook, T. Johannessen, A. Olsen, R. Bellerby, C. S. Wong, B. Delille, N. R. Bates and H. J. W. de Baar (2009). "Climatological mean and decadal change in surface ocean pCO_2, and net sea-air CO_2 flux over the global oceans." Deep-Sea Research Part I-Oceanographic Research Papers 56(11): 2075-2076.

Voss, K. J., Balch, W. M., & Kilpatrick, K. A. (1998). Scattering and attenuation properties of Emiliania huxleyi cells and their detached coccoliths. *Limnology and Oceanography*, *43*(5), 870–876. https://doi.org/10.4319/lo.1998.43.5.0870

Wanninkhof, R. (2014). "Relationship between wind speed and gas exchange over the ocean revisited." Limnology and Oceanography-Methods 12: 351-362.

Watts, J., T. G. Bell, K. Anderson, B. J. Butterworth, S. Miller, B. Else and J. Shutler (2022). "Impact of sea ice on air-sea CO_2 exchange – a critical review of polar eddy covariance studies." Progress in Oceanography: 102741.

Woolf, D. K., P. E. Land, J. D. Shutler, L. M. Goddijn-Murphy and C. J. Donlon (2016). "On the calculation of air-sea fluxes of CO_2 in the presence of temperature and salinity gradients." Journal of Geophysical Research: Oceans 121(2): 1229-1248.